Universidade de Aveiro Departamento de Física
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THERMALISATION AND ENTROPY IN HEISENBERG SPIN CHAINS

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dissertação apresentada à Universidade de Aveiro para cumprimento dos requisitos necessários à obtenção do grau de Mestre em Física, realizada sob a orientação científica do Professor Doutor Renato Renner, da ETH Zürich, e co-orientação do Professor Doutor Ricardo Dias, Professor auxiliar do Departamento de Física da Universidade de Aveiro

o júri

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palavras-chave

Termalização, equilíbrio, entropia, informação quântica, modelo de Heisenberg.

resumo

Este projecto tem como objectivo estudar o comportamento de medidas de entropia quântica em pequenos sistemas quânticos, de forma a se obter uma intuição sobre o assunto que veja a ser útil para um futuro projecto dedicado ao desenvolvimento de uma termodinâmica para pequenos sistemas quânticos baseada em entropias quânticas.

Mostramos como modelar sistemas quânticos que interagem entre si.

Introduzimos a noção de entropia quântica e discutimos o significado físico de algumas medidas de entropia, bem como as relações entre si.

Apresentamos uma abordagem do ponto de vista da informação quântica ao problema da termalização e equilíbrio. De seguida introduzimos e discutimos os sistemas modelo estudados, cadeias de spin de Heisenberg.

Para contribuir para esta linha de trabalho, desenvolvemos e executamos simulações numéricas nestas cadeias de spin, de forma a estudar o comportamento de várias medidas de entropia à medida que pequenos subsistemas termalizavam.

Entre outras coisas, concluímos que as diferentes medidas de entropia apresentam diferentes tempos de saturação. Apenas a medida de entropia mais lenta constitui um indicador adequado acerca do estado de termalização do sistema.

keywords

Thermalisation, equilibrium, entropy, quantum information, Heisenberg spin chains.

abstract

The goal of this project is to study the behaviour of quantum entropy measures in small quantum systems, in order to get an intuition for the subject that may help to orientate a future project dedicated to the development of a thermodynamic theory of small quantum systems based on quantum entropies. We show how to model composite (in particular interacting) quantum systems. We introduce the notion of quantum entropy and discuss the physical meaning of some entropy measures and the relations between them.

We present a quantum-information framework to the phenomena of thermalisation and equilibration and recall state-of-the-art results in this topic. Then we introduce the toy systems of study, Heisenberg spin chains, from the most basic principles of spin and exchange interaction. We discuss their physical meaning and how they behave under the action of the XXZ Hamiltonian. To contribute to that body of work we finally develop and perform numerical simulations in those spin chains in order to study the behaviour of several entropy measures as small systems thermalised.

Amongst other things, we find that distinct entropy measures saturate at different times. Only the slowest of these measures is appropriate to indicate whether a system has equilibrated.

Contents

Chapter 1

Introduction

In this project we study the thermodynamics of small systems using tools from quantum information. The thermodynamic entropy measure S that makes sense for large systems that can be described by some macroscopic parameters like temperature and pressure. Quantum information theory has introduced several other entropy measures with other operational meanings. For large and uncorrelated systems, these new entropies coincide with S. However, as we move to smaller quantum systems (for instance, a gas with less than a thousand particles) these entropies show different behaviour and one needs to think more carefully about which one(s) to use.

Here, we study the behaviour of some of these systems, spin chains, and try to look for thermodynamic behaviour. In particular, we try to understand which entropy measure or measures better describe the small systems studied and have properties that are similar to those of the macroscopic entropy (eg. the second law of thermodynamics).

In chapter two we see how to describe a quantum system using density matrices and how to model the interaction between a small system and a bath. In the third chapter we introduce several measures of quantum entropy as well as the concept of purity. The relations between these measures is addressed. The evolution in time of these quantum measures is discussed. In the fourth chapter we introduce a quantum-information approach to the phenomena of equilibrium and thermalisation. The toy model used in this thesis in order to study the thermodynamics of small quantum systems is the one-dimensional Heisenberg model. In chapter five the basis of this model is presented. The chapter six is dedicated to numerical results of the quantum entropy measures in the anisotropic Heisenberg model, the XXZ Hamiltonian. Finally, in the last chapter the main conclusions are presented.

Chapter 2

Composite quantum systems

In this chapter we introduce basic concepts and tools that are necessary to deal with interacting quantum systems. We begin by presenting the formalism of density matrices and a statistical interpretation for these objects. We will show how to use them to represent quantum states in composed systems and how to extract the state of one subsystem by means of partial trace, and then we recall how time evolution and measurements are modelled in quantum theory. We then introduce the trace distance, a measure of similarity between quantum states, and justify its importance. Finally we present two approaches to the problem of modelling a small quantum system that interacts with a heat bath – a recurrent topic in thermodynamics. Results obtained from these approaches will be addressed in chapter four. We do not yet refer to any concrete systems, as that will be done in chapter six.

2.1 Density matrices

When one is not studying a single isolated system but rather the interaction between several quantum systems, it is useful to describe them in the language of density matrices. Density matrices express the probability distribution of the possible states in which a quantum system may be found through measurements. Density matrices allow us to quantify correlations between systems and the entropy of subsystems of the global system. They are also essential to study the evolution and measurements performed on a subsystem.

Mathematically, a density operator is a normalised Hermitian non-negative operator on a Hilbert space, i.e., with trace one and non-negative eigenvalues. A density matrix ρ in a finite Hilbert space can be diagonalised and written as

$$\rho = \sum_x \lambda_x |x\rangle\langle x|, \tag{2.1}$$

where $\{\lambda_x\}_x$ are the matrix eigenvalues and $\{|x\rangle\}_x$ the eigenvectors.

Since the eigenvalues sum up to one, they form a probability distribution, where λ_x may be seen as the probability that the pure state $|x\rangle$ occurs. A density matrix is said to be *pure* if there is only one such possible state, i.e., if the matrix has the form $\rho = |\phi\rangle\langle\phi|$ or, equivalently, if $\mathrm{Tr}(\rho^2) = 1$. In this case, one has as much information as possible about the state of the system represented by the density matrix. Otherwise, if there is more than one non-zero eigenvalue, we say that the system is in a *mixed* state. In particular, if all the states are equally likely – in which case we have no information about the system – the density matrix is said to be *fully mixed*, and has the form $\rho = \frac{1}{d}\mathbb{1}_d$, where $\mathbb{1}_d$ is the identity matrix on a d-dimensional Hilbert space.

2.2 Partial trace

We now consider a system formed by two subsystems A and B, with a density matrix ρ_{AB} that is defined on the composed Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$:

$$\rho_{AB} = \sum_{x,y} \sum_{m,n} \alpha_{xm}^{yn} \left(|x\rangle \otimes |m\rangle\right) \left(\langle y| \otimes \langle n|\right). \tag{2.2}$$

From now on we will denote composed states of the form $|x\rangle \otimes |m\rangle$ by $|x\rangle|m\rangle$ or simply $|xm\rangle$. The (usually mixed) state of one of the subsystems can be obtained by *tracing out* the other. This is done by means of a *partial trace*,

$$\rho_A = \mathrm{Tr}_B(\rho_{AB}). \tag{2.3}$$

The resulting *reduced density matrix* of subsystem A is

$$\rho_A = \sum_{x,y} \alpha_x^y |x\rangle\langle y|, \tag{2.4}$$

where the coefficients α_x^y are given by the sum of the coefficients of the terms $|xm\rangle\langle ym|$ over all possible states $|m\rangle$ of subsystem B,

$$\alpha_x^y = \sum_m \alpha_{xm}^{ym}. \tag{2.5}$$

In general, the partial trace of a composed operator $S_A \otimes S_B$ is defined as

$$\mathrm{Tr}_B(S_A \otimes S_B) = \mathrm{Tr}(S_B) S_A, \tag{2.6}$$

where $\mathrm{Tr}(S)$ is the usual trace. Note that

$$\mathrm{Tr}(S_A \otimes S_B) = \mathrm{Tr}(\mathrm{Tr}_B(S_A \otimes S_B)) = \mathrm{Tr}(\mathrm{Tr}_A(S_A \otimes S_B)). \tag{2.7}$$

To make this cleaner we give an example. Consider a system with two qubits A and B, each one of them with two accessible states $|0\rangle$ and $|1\rangle$. If the system is prepared with the global pure state

$$|\phi\rangle = \frac{1}{\sqrt{3}} \left(|0_A 0_B\rangle + |1_A 0_B\rangle + |1_A 1_B\rangle \right)$$

then the density matrix of the system is given by $\rho_{AB} = |\Phi_{AB}\rangle\langle\Phi_{AB}|$ or, in the basis $\{|0_A 0_B\rangle, |0_A 1_B\rangle, |1_A 0_B\rangle, |1_A 1_B\rangle\}$, by

$$\rho_{AB} = \frac{1}{3} \begin{pmatrix} 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}.$$

This matrix has eigenvalues $\{1, 0, 0, 0\}$, with the eigenvector of the only non-zero eigenvalue being of course $|\phi\rangle$.

To obtain the reduced density matrix of the subsystem A, one has to evaluate the sum of Eq. 2.5. For instance, the coefficient α_0^1 that corresponds to the mixture $|0_A\rangle\langle 1_A|$ (in blue ahead) is given by the sum of the coefficients of the terms corresponding to $|0_A 0_B\rangle\langle 1_A 0_B|$ and $|0_A 1_B\rangle\langle 1_A 1_B|$ of the original density matrix. In the basis $\{|0_A\rangle, |1_A\rangle\}$, the reduced state is represented by the matrix

$$\rho_A = \frac{1}{3} \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}.$$

The colours indicate the elements of the ρ_{AB} that were summed up to each of the entries of ρ_A. Since the basis of the global system was nicely ordered, each element of the new one was calculated by the trace of the 2×2 "submatrix" that is in the corner of the original matrix indicated by the position of the desired element in the new one. The resulting state is mixed, as the reduced density matrix has two non-zero eigenvalues.

2.3 Evolution

A quantum state $\rho(t)$ evolves under unitary operators as

$$\rho(t_1) = U \rho(t_0) U^\dagger. \tag{2.8}$$

In particular, if the total system is governed by the time-independent Hamiltonian $\mathcal{H}_{AB}$, as will happen in this work, the density matrix at time t is given by

$$\rho_{AB}(t) = e^{-i\mathcal{H}_{AB}t} \rho_{AB}(0) e^{+i\mathcal{H}_{AB}t}, \tag{2.9}$$

setting $\hbar = 1$.

2.4 Measurements

A measurement performed in a quantum state defined on a Hilbert space $\mathcal{H}_A$ is described by a Hermitian operator S_A whose eigenvalues $\{x\}_x$ are the possible outcomes of the measurement. The operator may be written by spectral decomposition as $\sum_x xP_x$, where the projectors P_x respect the property $\sum_x P_x = \mathbb{1}$.

In order to perform the measurement represented by S_A on a state ρ_{AB} that is defined on a space $\mathcal{H}_A \otimes \mathcal{H}_B$ one may either apply it directly as $S_A \otimes \mathbb{1}_B$ on ρ_{AB} and then trace out the system B or start by tracing out B and then apply S_A on $\rho_A = \mathrm{Tr}_B(\rho_{AB})$. Regardless of the method chosen to apply the measurement, the final state of the system and the probability distribution of the possible outcomes are the same: the probability of obtaining x in the measurement is given by

$$\begin{aligned} \mathcal{P}(x|\rho_{AB}) &= \mathrm{Tr}\left(\left[P_x \otimes \mathbb{1}_B\right] \rho_{AB}\right) \\ &= \mathrm{Tr}\left(P_x \rho_A\right), \end{aligned} \tag{2.10}$$

and after the measurement the system collapses to the state

$$\rho_{AB}^x = \frac{1}{\mathcal{P}(x|\rho_{AB})} \left[P_x \otimes \mathbb{1}_B\right] \rho_{AB} \left[P_x \otimes \mathbb{1}_B\right]. \tag{2.11}$$

2.5 Trace distance

A *distance* between two quantum states is a way of quantifying how close, or similar, the states are. There exist several distance measures defined on density matrices, which are more or less useful according to the criteria used to distinguish the quantum states. Here we will use the *trace distance*, defined as

$$\delta(\rho_1, \rho_2) = \frac{1}{2}\mathrm{Tr}|\rho_1 - \rho_2|, \tag{2.12}$$

where $|A| = \sqrt{A^\dagger A}$ is the positive square root of $A^\dagger A$. This distance is zero for equal density matrices and has the maximum value of one for different pure states.

The trace distance is a very general and powerful measure as it maximises the classical statistical distance D between measurement results that may be obtained by applying any measurement to the two states,

$$\delta(\rho_1, \rho_2) = \max_O D(\mathcal{P}_1, \mathcal{P}_2) \tag{2.13}$$

where $\mathcal{P}_1$ and $\mathcal{P}_2$ are the probability distributions that are obtained by applying the observable O to states ρ_1 and ρ_2 respectively (15; 10).

In particular, given two different states with known density matrices ρ_1 and ρ_2 and the possibility of performing a single measurement in one of them at random, the probability of correctly guessing which state was measured is, in the best possible case, given

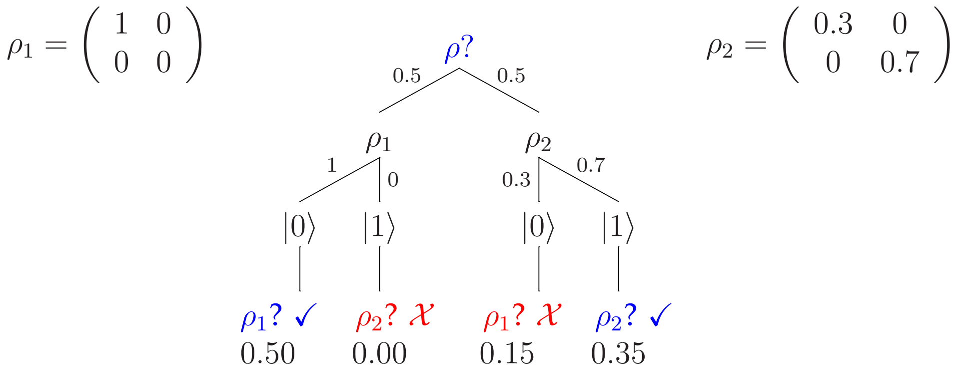

Figure 2.1: Trying to distinguish two quantum states through a single measurement: a basic example. The states ρ_1 and ρ_2 are represented in the basis $\{|0\rangle, |1\rangle\}$. The optimal strategy here is to measure one of them at random in that basis (with the observable $\mathbb{1}$) and then risk guessing that the state measured is the one that was more likely to have the outcome observed: in this case ρ_1 if the state collapses to $|0\rangle$ and ρ_2 if it collapses to $|1\rangle$. Here, the probability $\mathcal{P}_{\checkmark}$ of guessing correctly is given by the sum $\mathcal{P}(\text{outcome is } |0\rangle \text{ and state is } \rho_1) + \mathcal{P}(\text{outcome is } |1\rangle \text{ and state is } \rho_2) = 0.50 + 0.35 = 0.85$. The trace distance between the states is $\delta(\rho_1, \rho_2) = 0.7$. The rule $\mathcal{P}_{\checkmark}(\rho_1, \rho_2) = \frac{1}{2}(1 + \delta(\rho_1, \rho_2))$ applies here.

by (3; 10)

$$\mathcal{P}_{\checkmark}(\rho_1, \rho_2) = \frac{1}{2}\left(1 + \delta(\rho_1, \rho_2)\right). \tag{2.14}$$

A simple example of this process is given in Fig. 2.5.

2.6 The system and the bath

The interaction between a subsystem and a heat bath, and the consequent equilibration and thermalisation of the subsystem, are extensively studied phenomena in thermodynamics. The heat bath is usually described as a system that is so large compared to the subsystem of interest that the interaction with the subsystem does not affect its macroscopic parameters such as temperature, pressure and total energy. There have been some attempts in the quantum information community to model the interaction between a quantum system and a bath. We introduce here two opposite approaches.

In the first one, followed, for instance, by Valerio Scarani (16), the bath is characterised entirely by the interaction with the subsystem. Instead of stating directly that the bath is large, the interaction between subsystem and bath is modelled with properties that are expected to be a natural consequence of the fact that the bath is much bigger than the subsystem. One example of such properties is the assumption that each particle of the bath only interacts with the system at most once, which would make sense probabilistically if it were composed of many discrete particles. This property ensures that the bath has effectively no memory, i.e., is the same for each interaction with the subsystem. Also, variations in the energy of the particles of the bath caused by such interactions are very faint and scattered across the bath, and thus do not influence its macroscopic parameters. It is also commonly specified whether the particles of the bath may interact with each other or with some external field. Adjusting these properties, the bath may be bound to an essentially static state. In this type of model it is established from the beginning which part of the system is the subsystem of interest and which is the bath, the latter being defined by its impact on the former.

Popescu et al. (11; 8) follow a very different approach. While the properties of both the system and the bath are left completely unbounded and general (in fact, the bath may be any subsystem of the total system), a restriction is made on the Hamiltonian that governs the total system, namely that it is fully interactive – which is expressed mathematically as not having degenerate energy gaps. Under these conditions they prove that nearly any subsystem that is much smaller than the total system will equilibrate, while the remaining subsystem behaves like a bath. We will discuss this approach and one main result in chapter four.

Let us make a quick analogy to better illustrate the difference between these two approaches. Suppose that two social scientists want to study the behaviour and evolution of a person inserted in a stressful society but use different scientific methods. The first scientist picks a child and constructs an artificial society with actors around him, much like the world of *The Truman Show*, defined only in function of the person of interest. The actors are told to behave near that person as if they had stressful jobs and were always upset with the traffic. The other expert says simply that nearly any random single inhabitant of any city that is large enough and where people interact at least a bit with each other is a good subject of study, since from the point of view of that person the rest of the inhabitants of the city behave as a stressful society.

The first approach is useful mostly in concrete cases where it is known how the subsystem behaves in contact with the bath so that the interaction may be modelled precisely without the need for simulating a large bath. On the other hand, the second method is more natural and general, yielding more powerful results, as we will see in the chapter dedicated to thermalisation.

Chapter 3

Quantum entropy measures

Entropy is a measure of the randomness of a system, or equivalently of the uncertainty of an observer about it. The quantum entropy measures are operators that act on the density matrix ρ that describes a system as seen by an observer and express how flat the probability distribution defined by its eigenvalues $\{\lambda_i\}_i$ is.

In this chapter we will introduce and discuss several entropy measures that will be used in the simulations of chapter six.

From now on all the logarithms are binary, so we will write $\log x \equiv \log_2 x$ to simplify notation. Also, when computing entropy measures we will adopt the convention that $0 \log 0 = 0$.

3.1 Max-entropy

One way of quantifying how much information we may extract from a quantum state defined in, say, N qubits is by answering the following question: *how many qubits can be made fully known by applying only reversible operations to the state?* The number of qubits that cannot be fully determined this way we will call the max-entropy – by definition a measure of uncertainty about a quantum state. The fact that the allowed operations are reversible ensures that we may not modify the state by, for instance, measuring some of the qubits. After determining the maximum number of qubits possible we must be able to restore the state its initial form. In quantum theory, a reversible operation is represented by an unitary operator.

As an example, consider the state

$$\rho = \frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|11\rangle\langle 11|. \tag{3.1}$$

In this state only one of the qubits is unknown – once we measure one of them we know immediately the state of the other. However, we do not know *a priori* the state of either of the qubits. To this state the unitary operator controlled-not, CNOT , may be applied.

This operator flips the second qubit if the first one is $|1\rangle$ and does nothing otherwise:

$$\text{CNOT } = |00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 11| + |11\rangle\langle 10| \tag{3.2}$$

obtaining the state

$$\begin{aligned}\text{CNOT } \rho \,\text{CNOT }^\dagger &= \frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|10\rangle\langle 10| \\ &= \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right) \otimes |0\rangle\langle 0|, \end{aligned} \tag{3.3}$$

wherein the second qubit is in the pure state $|0\rangle\langle 0|$ (therefore being always known) and the first one is fully mixed. In this case, the answer to our question is "one".

We will now generalise this problem to all density matrices that are diagonal in the canonical basis, $\{|0\rangle, |1\rangle\}^{\otimes n}$. The solution we present is valid in general but it is easier to visualise for matrices that are diagonal in this basis. Ordering the states by their binary representation, e.g. $|5\rangle \equiv |101\rangle$, the density matrix may be written as

$$\rho = \sum_i^{2^N} \alpha_i |i\rangle\langle i|, \qquad \sum_i \alpha_i = 1 \wedge \forall \alpha_i > 0. \tag{3.4}$$

Permutations, on the other hand, are operators of the form

$$\Pi = \sum_i^{2^N} |i\rangle\langle k_i|, \qquad |k_i\rangle = |k_j\rangle \Leftrightarrow |i\rangle = |j\rangle, \tag{3.5}$$

i.e., whose representation in the canonical basis has only one entry of 1 in each row an column, like the CNOT operator. These operators are naturally unitary, since

$$\begin{aligned}\Pi\Pi^\dagger &= \left(\sum_i |i\rangle\langle k_i|\right)\left(\sum_j |k_j\rangle\langle j|\right) \\ &= \sum_{i,j} |i\rangle\langle k_i|k_j\rangle\langle j| \\ &= \sum_{i,j} |i\rangle\delta_{i,j}\langle j| = \mathbb{1}.\end{aligned}$$

When applied (as $\Pi\rho\Pi^\dagger$) to a diagonal matrix ρ, permutations simply swap the entries in the diagonal. For any diagonalised density matrix ρ with $\Lambda = \operatorname{rank}(\rho)$ non-zero eigenvalues $\{\alpha_i\}_i$ there is a permutation Π such that

$$\Pi\rho\Pi^\dagger = \sum_i^{\Lambda} \beta_i |i\rangle\langle i|, \tag{3.6}$$

with $\beta_i = \alpha_j$ for some $j \leq 2^N$.

This representation allows us to fully know the first $N - \log \text{rank}\ (\rho)$ qubits, that are set to $|0\rangle$. For instance, for $N = 4$ and $\text{rank}\ (\rho) = 4$ we have

$$\begin{aligned}\Pi\rho\Pi^\dagger &= \beta_1|0000\rangle\langle 0000| + \beta_2|0001\rangle\langle 0001| + \beta_3|0010\rangle\langle 0010| + \beta_4|0011\rangle\langle 0011| \\ &= |00\rangle\langle 00| \otimes (\beta_1|00\rangle\langle 00| + \beta_2|01\rangle\langle 01| + \beta_3|10\rangle\langle 10| + \beta_4|11\rangle\langle 11|)\,.\end{aligned}$$

The first two qubits are fully known while the other two are in a mixed state. The max-entropy of a quantum state is therefore given by

$$H_{\max}(\rho) = \log \text{rank}\ (\rho), \tag{3.7}$$

and represents the number of uncertain qubits of the state.

3.2 Min-entropy

While the max-entropy gives us the number of not fully known qubits of a quantum state, which may be biased in any way, the min-entropy gives in particular sense the number of uniformly random qubits, n_U. It depends only on the maximum eigenvalue of the density matrix,

$$H_{\min}(\rho) = -\log \lambda_{\max}, \qquad \lambda_{\max} = \max\{\lambda_i\}_i \quad \text{eigenvalues of } \rho. \tag{3.8}$$

We will show briefly that the min-entropy is always greater or equal than the number of uniformly random qubits $H_{\min} \geq n_U$. The proof that $H_{\min} \approx n_U$ is given by the leftover hash-lemma (5).

Given a quantum state ρ_{AB} defined in a composite system $\mathcal{H}_A \otimes \mathcal{H}_B$, we say that the state is uniformly random in the subsystem $\mathcal{H}_A$ if $\rho_A = \text{Tr}_B(\rho_{AB}) = \frac{1}{d}\mathbb{1}$ is fully mixed.

Let $\lambda_{\max}$ be the maximum eigenvalue of the density matrix ρ, defined in a system $\mathcal{H}$ that is composed of N qubits.

By the definition of the partial trace, the maximum eigenvalue of the reduced density matrix obtained by partial trace of ρ is at least as large as $\lambda_{\max}$. The largest mixed reduced state possible is then $\lambda_{\max}\mathbb{1}$, which implies that the dimension of that state is at most $d = \frac{1}{\lambda_{\max}}$.

Since a system of dimension d is encoded by $\log d$ qubits we obtain the desired result: the maximum number of totally random qubits is $n_U = -\log \lambda_{\max} = H_{\min}(\rho)$.

3.3 Von Neumann entropy

The Von Neumann entropy is the most commonly used entropy in quantum information (18). It is given by

$$\begin{aligned}H(\rho) &= -\text{Tr}(\rho \log \rho) \\ &= -\sum_i \lambda_i \log \lambda_i, \qquad \{\lambda_i\}_i \quad \text{eigenvalues of } \rho.\end{aligned} \tag{3.9}$$

It has an asymptotic interpretation as the mean entropy of an event that is repeated independently many times – or of a quantum system composed of many independent subsystems. Even though this entropy has no intuitive physical meaning for processes that are performed only a few times or for highly correlated systems, it is very popular in the quantum information community and was used to produce many important results in quantum cryptography, communication and information theory.

3.4 Smooth min- and max-entropies

Smooth min and max-entropies were introduced recently by Renato Renner and Stefan Wolf (13) partly as a response to the asymptotic-only interpretation of the Von Neumann entropy. Smooth entropies allow some error tolerance on the density matrix and are generally continuous on the probability distribution defined by its eigenvalues (unlike, for instance, the max-entropy).

Let $\mathcal{B}^\varepsilon(\rho)$ be the open ball of the states that are ε- close to ρ with respect to the trace distance.

The smooth min-entropy is defined as

$$H^\varepsilon_{\min}(\rho) = \sup_{\rho' \in \mathcal{B}^\varepsilon(\rho)} H_{\min}(\rho'), \tag{3.10}$$

and the smooth max-entropy is defined as

$$H^\varepsilon_{\max}(\rho) = \inf_{\rho' \in \mathcal{B}^\varepsilon(\rho)} H_{\max}(\rho'). \tag{3.11}$$

In Hilbert spaces of finite dimension, $\sup$ and $\inf$ may be replaced by $\max$ and $\min$ respectively.

3.5 Other Rényi entropies

A quantum Rényi entropy of order α is defined as

$$H_\alpha(\rho) = \frac{1}{1-\alpha} \log \mathrm{Tr}\rho^\alpha. \tag{3.12}$$

The quantum $\varepsilon-$smooth Rényi entropy of order α is defined as

$$H_\alpha(\rho) = \frac{1}{1-\alpha} \inf_{\rho' \in \mathcal{B}^\varepsilon(\rho)} \log \mathrm{Tr}\rho^\alpha. \tag{3.13}$$

One may distinguish two main families of Rényi entropies: those of order $\alpha > 1$, which behave like the smooth min-entropy, which arises in the limit $\alpha \to +\infty$; and the ones of order $\alpha < 1$ which resemble the smooth max-entropy that corresponds to $\alpha = 0$. The Von Neumann entropy is obtained in the limit case $\alpha = 1$.

3.6 Purity and effective dimension

Another important quantity in quantum information is the so-called *purity* of a density matrix, given by

$$P = \mathrm{Tr}(\rho^2). \tag{3.14}$$

The purity will be used here to define the so-called effective dimension of a system that gives a measure of the number of states through which the system goes more often. This quantity is used for instance by Linden et al. (8),

$$d_{\text{eff}} = \frac{1}{\mathrm{Tr}(\rho^2)}. \tag{3.15}$$

Note that $d_{\text{eff}} = 2^{H_2}$. Other *dimensions* of slightly different meanings may be obtained for all the Rényi entropies as $d_\alpha = 2^{H_\alpha}$

3.7 General properties of quantum entropies

All (non-conditional[1]) Rényi entropies are non-negative, with a minimum value of 0 for pure states and a maximum of $\log n$ for fully mixed states of dimension n.

The entropy of a closed system (no matter which particular measure of entropy) is time invariant. The reason for this is that the entropy measures depend uniquely on the eigenvalues of the density matrix and these are a constant of motion. This follows from the fact that evolution under an unitary may be seen as a change of basis and the eigenvalues of a matrix are invariant under such operations. However, the entropy of a given subsystem may change under time – and usually does so.

In the asymptotic limit for uncorrelated systems both min- and max-smooth entropies converge to the Von Neumann entropy – see eg.(17),

$$\forall\rho \quad \lim_{\varepsilon\to 0}\lim_{n\to\infty} \frac{H^{\varepsilon}_{\min}(\rho^{\otimes n})}{n} = \lim_{\varepsilon\to 0}\lim_{n\to\infty} \frac{H^{\varepsilon}_{\min}(\rho^{\otimes n})}{n} = H(\rho). \tag{3.16}$$

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[1] We will not deal with conditional entropies in this work.

Chapter 4

Equilibration and thermalisation

In this chapter we follow the approach of Popescu et al. (11; 8) to the thermalisation of quantum systems. We start by introducing the notion of thermalisation and some criteria to evaluate how close a system is to being thermalised. We will use these criteria in our simulations – see chapter six. Finally we present recent results on equilibration of very general systems (8).

4.1 Definition of thermalisation

Given a Hilbert space $\mathcal{H}$ and a decomposition $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$ (with $d_S = \dim \mathcal{H}_S \ll d_B = \dim \mathcal{H}_B$), one says that the subsystem S has *thermalised* if it has (1) reached an equilibrium state $\boldsymbol{\rho}_S^{\mathbf{eq}}$ that is (2) independent of the initial state of the subsystem ρ_S^0 and (3) independent of the exact state of the bath, depending only on macroscopic quantities that are averaged over the bath, such as *temperature*.

Moreover, the equilibrium state is expected to (4) have the Boltzmannian form $\rho_S^\beta = \frac{\exp(-H_S\beta)}{Z}$, where Z is the partition function calculated for the Hamiltonian H_S that governs the time evolution of the subsystem[1] and β is a real constant defined by the macroscopic parameters of the bath.

4.2 Preliminary concepts

The average $\langle f(x)\rangle_{x_1,\cdots,x_n}$ denotes the average over *all possible values* of the variables $x_1, \cdots, x_n$. For instance $\langle \rho(t)\rangle_t$ is the average of the state $\rho(t)$ from $t = 0$ to $t = \infty$.

Let $\Lambda = \{\Lambda_1, \Lambda_2, \cdots, \Lambda_N\}$ be the macroscopic parameters (such as temperature, volume, pressure, etc.) that we use to characterise the bath, and $\lambda = \{\lambda_1, \lambda_2, \cdots, \lambda_N\}$ a set of instances of those parameters.

We denote by $\Omega|_{\Lambda=\lambda}$ the set of states ρ_{SB} of the total state for which the reduced state of the bath $\rho_B = \mathrm{Tr}_S(\rho_{SB})$ verifies $\Lambda_1 = \lambda_1 \wedge \Lambda_2 = \lambda_2 \wedge \cdots \wedge \Lambda_N = \lambda_N$.

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[1] It is not clear how this Hamiltonian may be defined for all cases.

Let $U(t_1 - t_0)$ be the unitary that governs the time evolution of the global system from the instant $t = t_0$ to $t = t_1$, such that the global state of the system at time t is given by $\rho_{SB}(t) = U(t)\rho_{SB}^0 U(t)^\dagger$, for an initial state ρ_{SB}^0. The state of the subsystem S at time t is given naturally by $\rho_S(t) = \mathrm{Tr}_B(\rho_{SB}(t))$.

We further denote by $\boldsymbol{\rho}_S^{\mathbf{eq}}(\rho_{SB}^0)$ the equilibrium state of the subsystem S that is defined as the time average of all the states the subsystem goes through during infinite time, obtained after evolution from the initial global state ρ_{SB}^0,

$$\boldsymbol{\rho}_S^{\mathbf{eq}}(\rho_{SB}^0) = \langle \rho_S(t) \rangle_t, \qquad \rho_S(t) = \mathrm{Tr}_B(U(t)\rho_{SB}^0 U(t)^\dagger). \tag{4.1}$$

Whenever the knowledge of the initial global system ρ_{SB}^0 is not necessary we will denote the equilibrium state simply by $\boldsymbol{\rho}_S^{\mathbf{eq}}$.

4.3 Evaluating the thermalisation of a system

We now define a way of quantifying the four conditions specified above, based on the trace distance δ between states. The quantities $D_1 - D_4$ that we introduce must be as small as possible to ensure that the subsystem thermalises.

A good way of verifying if a subsystem equilibrates is to measure how much it deviates from the equilibrium state on average:

$$D_1 = \langle \delta\left(\rho(t), \boldsymbol{\rho}_S^{\mathbf{eq}}\right) \rangle_t \tag{4.2}$$

cannot be big. Conditions (2) and (3) are satisfied if all global states that have the same macroscopic parameters conditions lead to the same equilibrium state of the subsystem, i.e.,

$$D_{2,3} = \langle \quad \langle \delta\left(\boldsymbol{\rho}_S^{\mathbf{eq}}(\rho_1), \boldsymbol{\rho}_S^{\mathbf{eq}}(\rho_2)\right) \rangle_{\rho_1,\rho_2}, \quad \rho_1, \rho_2 \in \Omega|_{\Lambda=\lambda} \quad \rangle_\lambda \tag{4.3}$$

must be small. Finally, the last condition simply implies that the distance between the equilibrium state obtained and the Boltzmannian one,

$$D_4 = \delta(\boldsymbol{\rho}_S^{\mathbf{eq}}, \rho_S^\beta) \tag{4.4}$$

is small as well.

4.4 Condition for equilibration

In (8), the authors address the thermalisation of quantum systems in a very general way. The form of the composed Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_B$ is left mostly unbounded, with a single condition: that the Hamiltonian that governs the total system has non-degenerate energy gaps. This condition ensures that the Hamiltonian is fully interactive without imposing any other restrictions. In fact, adding an arbitrarily small random perturbation to a Hamiltonian breaks the gaps degeneracy.

In these conditions, they prove that "whenever the state of the total system goes through any distinct states, any small subsystem equilibrates", i.e.,

$$\langle \delta \left(\rho(t), \boldsymbol{\rho}_S^{\mathbf{eq}} \right) \rangle_t \leq \frac{1}{2}\sqrt{\frac{d_S}{d_{\text{eff}}(\boldsymbol{\rho}_B^{\mathbf{eq}})}} \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d_{\text{eff}}(\boldsymbol{\rho}_{SB}^{\mathbf{eq}})}}, \tag{4.5}$$

that the distance to equilibrium of the subsystem is bounded by a function of the relative size of subsystem compared to the effective size of the total system.

Chapter 5

Spin chains

Spin chains are simple toy systems that are easy to study and a good starting point for testing the thermodynamic behaviour of finite systems. In this chapter we introduce the interaction between spins and the Heisenberg model that will be used in the numerical simulations. We will also review some known results regarding thermalisation of spin chains.

5.1 Spin

Matter carries certain properties such as charge, mass, wave number or momentum that allow us to distinguish between particles and types of particles and ultimately to tell the difference between a peach tree and a compass. One of the least intuitive of these properties is the *spin*, often referred to as the intrinsic angular momentum.

For each type of particle, the spin vector $\mathbf{S}$ is characterized by a quantum number s: the magnitude of spin is $\sqrt{s(s+1)}\hbar$ and, for each particle of that kind, the value of spin along any direction is given by $m_s\hbar$, with the quantum number $|m_s| \leq s$ such that $s - m_s$ is an integer. From spin arises a magnetic moment: $\boldsymbol{\mu}_S = g\frac{q}{2m}\mathbf{S}$, where q is the charge of the particle, m its mass and g the g-factor, a dimensionless constant predicted by QED. A particle with magnetic moment $\boldsymbol{\mu}_S$ in the presence of a magnetic field B has potential energy $E = -\boldsymbol{\mu} \cdot \mathbf{B}$.

Electrons are known as spin $\frac{1}{2}$ particles because they have $s = \frac{1}{2}$. The amplitude of spin is therefore $\frac{\sqrt{3}}{2}\hbar$ and any of its components must either take the value $+\frac{\hbar}{2}$ (*spin up*, if spin is measured along the z axis) or $-\frac{\hbar}{2}$ (*spin down*). Also in the case of electrons, the g-factor is close to 2 and it is convenient to define a new constant, the *Bohr magneton*, as $\mu_B = \frac{e\hbar}{2m_e}$. The magnitude of the magnetic moment is then approximately $\frac{\sqrt{3}}{2}\mu_B$ and the projections along an axis are $\mp\mu_B$ for spin up and down. The energy of an electron in a magnetic field is $E \approx \pm\mu_B B$. These properties are summarised in Table 5.1.

In order to formalise the previous concepts, let us introduce the Pauli spin matrices,

quantum numbers	*in general*	*electrons*
s	> 0	$1/2$
m_s	$-s, -s+1, ..., s-1, s$	$\pm 1/2$
spin		
magnitude	$\sqrt{s(s+1)}\hbar$	$\sqrt{3}\hbar/2$
components	$m_s\hbar$	$\pm \hbar/2$
magnetic momentum		
magnitude	$\sqrt{s(s+1)}g\hbar\|q\|/2m$	$\approx \sqrt{3}\mu_B/2$
components	$m_s g\hbar q/2m$	$\approx \mp\mu_B$
energy	$-\boldsymbol{\mu}\cdot\mathbf{B}$	$\approx \pm\mu_B B$

	egvalue	*egstates*
S^x	$+1/2$	$1/\sqrt{2}(\|\uparrow\rangle + \|\downarrow\rangle)$
	$-1/2$	$1/\sqrt{2}(\|\uparrow\rangle - \|\downarrow\rangle)$
S^y	$+1/2$	$1/\sqrt{2}(\|\uparrow\rangle + i\|\downarrow\rangle)$
	$-1/2$	$1/\sqrt{2}(\|\uparrow\rangle - i\|\downarrow\rangle)$
S^z	$+1/2$	$\|\uparrow\rangle$
	$-1/2$	$\|\downarrow\rangle$
S^2	$+3/4$	$\alpha\|\uparrow\rangle + \beta\|\downarrow\rangle$

Table 5.1: Some properties of spin.

defined as

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.1}$$

These matrices allow us to study the behaviour of spin, since the spin operator for electrons is defined as $\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma} = \frac{1}{2}(\sigma^x, \sigma^y, \sigma^z)$. The components S^x, S^y and S^z of spin satisfy the commutation relations of angular momentum operators, $[S^l, S^m] = i\varepsilon_{lmn}S^n$ and $[S^2, S^l] = 0$, with $l, m, n \in \{x, y, z\}$ and $S^2 = (S^x)^2 + (S^y)^2 + (S^z)^2$.

The eigenvectors of the S^z operator are represented by $|\uparrow\rangle = \binom{1}{0}$ and $|\downarrow\rangle = \binom{0}{1}$ for eigenvalues $m_s = \frac{1}{2}$ and $m_s = -\frac{1}{2}$ respectively, working in units of $\hbar$ (or equivalently, setting $\hbar = 1$). The eigenstates of the spin $\frac{1}{2}$ operators (S^x, S^y, S^z and S^2) may be consulted in Table 5.1. One should note that any state $|\phi\rangle = \binom{\alpha}{\beta}$ is an eigenstate of S^2 with eigenvalue $\frac{1}{2}(\frac{1}{2}+1) = \frac{3}{4}$, since $S^2 = \frac{3}{4}\mathbb{1}$.

Other basic instruments usually required to deal with spins are the ladder, raising and lowering or flip operators, defined as

$$S_+ = S^x + iS^y, \tag{5.2}$$

$$S_- = S^x - iS^y. \tag{5.3}$$

From their matricial representations,

$$S_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad S_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{5.4}$$

it is clear that S_+ flips a spin from ↓ to ↑ and S_- does the opposite. Note that these operators are not Hermitian ($S_-^\dagger = S_+$ and vice versa).

5.2 Exchange interaction

We now consider interactions between spins, starting with the simplest example – the spins of only two interacting electrons a and b. The Hamiltonian that governs the *exchange interaction* is proportional to the inner product of the two spins,

$$\mathcal{H}_J = -J\mathbf{S}_a \cdot \mathbf{S}_b. \tag{5.5}$$

where J is the so-called *exchange constant*. The solution of this two-site Hamiltonian is relatively easy to achieve, as we will show. We can obtain $\mathbf{S}_a \cdot \mathbf{S}_b$ from the identity

$$(\mathbf{S}_a + \mathbf{S}_b)^2 = \mathbf{S}_a^2 + \mathbf{S}_b^2 + 2\mathbf{S}_a \cdot \mathbf{S}_b$$

The operator $\mathbf{S}_a^2$ acts only on the first qubit (more precisely, it represents the operator $\mathbf{S}_a^2 \otimes \mathbb{1}$). As we have seen, all states are eigenstates of this operator, with eigenvalue $\frac{3}{4}$. The same is valid for $\mathbf{S}_b^2$. Since the sum of spin vectors is still a spin operator, the spin amplitude $\mathbf{S}^2 = (\mathbf{S}_a + \mathbf{S}_b)^2$ has eigenvalues $s(s+1)$, with $|s_a - s_b| \leq s \leq s_a + s_b$ (again in integer steps). In the case of electrons, as $s_a = s_b = \frac{1}{2}$, s may only be 0 or 1. A state with total spin $s = 0$ is called a *singlet* state. There is only one such state (with $m_s = 0$), $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$. The amplitude of spin of this state is 0. There are three two-spin *triplet* states, with $s = 1$, spin amplitude 2 and $m_s = -1, 0, 1$. They are respectively $|\downarrow\downarrow\rangle$, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ and $|\uparrow\uparrow\rangle$. The eigenvalues of $\mathbf{S}_a \cdot \mathbf{S}_b$ are therefore

$$\begin{aligned}
\mathbf{S}_a \cdot \mathbf{S}_b &= -\frac{1}{2}(\mathbf{S}_a^2 + \mathbf{S}_b^2) + \frac{1}{2}(\mathbf{S}_a + \mathbf{S}_b)^2 \\
&= -\frac{1}{2}\left(\frac{3}{4} + \frac{3}{4}\right) + \frac{1}{2}\left\{ \begin{array}{l} 0, \text{ singlet} \\ 2, \text{ triplet} \end{array} \right. \\
&= \left\{ \begin{array}{ll} -{}^{3}\!/_{4}, & \text{singlet} \\ {}^{1}\!/_{4}, & \text{triplet,} \end{array} \right.
\end{aligned}$$

and the possible energy values of a two-spin system governed by the exchange interaction Hamiltonian are

$$\mathcal{H}_J = \left\{ \begin{array}{ll} +{}^{3}\!/_{4}J, & \text{singlet} \\ -{}^{1}\!/_{4}J, & \text{triplet.} \end{array} \right. \tag{5.6}$$

If J is negative, the singlet state is the ground state of the Hamiltonian and vice versa. As eigenstates these states are left untouched by time evolution. In order to visualise how the exchange interaction acts on other states it helps to write the Hamiltonian in terms of the flip operators,

$$\begin{aligned}
\mathcal{H}_J &= J\left(S_a^x S_b^x + S_a^y S_b^y + S_a^z S_b^z\right) \\
&= J\left(\frac{1}{2}\left[S_a^+ S_b^- + S_a^- S_b^+\right] + S_a^z S_b^z\right).
\end{aligned} \tag{5.7}$$

We are now ready to see what happens when we apply the Hamiltonian to other states. For instance,

$$\begin{aligned}\mathcal{H}_J|\downarrow\uparrow\rangle &= J\left(\frac{1}{2}\left[S_a^+S_b^-|\downarrow\uparrow\rangle + S_a^-S_b^+|\downarrow\uparrow\rangle\right] + S_a^zS_b^z|\downarrow\uparrow\rangle\right)\\ &= J\left(\frac{1}{2}\left[|\uparrow\downarrow\rangle + 0\right] + (-\frac{1}{2})(+\frac{1}{2})|\downarrow\uparrow\rangle\right),\end{aligned} \tag{5.8}$$

and, in the case of $|\uparrow\downarrow\rangle$,

$$\begin{aligned}\mathcal{H}_J|\uparrow\downarrow\rangle &= J\left(\frac{1}{2}\left[S_a^+S_b^-|\uparrow\downarrow\rangle + S_a^-S_b^+|\uparrow\downarrow\rangle\right] + S_a^zS_b^z|\uparrow\downarrow\rangle\right)\\ &= J\left(\frac{1}{2}\left[0 + |\downarrow\uparrow\rangle\right] + (-\frac{1}{2})(+\frac{1}{2})|\uparrow\downarrow\rangle\right).\end{aligned} \tag{5.9}$$

For pure states, time evolution processes as $|\phi(t)\rangle = e^{-i\mathcal{H}t}|\phi(0)\rangle$. This means that the initial state $|\downarrow\uparrow\rangle$ will evolve to a superposition of $|\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\rangle$. This scattering of a perturbation, a spin up in this case, through all the (two) sites is a manifestation of a more general phenomenon that we will find later.

5.3 Heisenberg model

Generalising the exchange interaction Hamiltonian to an arbitrary number of spins we obtain the Heisenberg model,

$$\mathcal{H} = -\sum_{(i,j)} \mathbf{J}_{ij}\mathbf{S}_i \cdot \mathbf{S}_j, \tag{5.10}$$

that sums over the exchange interaction of each pair of spins (i, j). In the presence of a magnetic field aligned, without loss of generality, along the z-direction, the potential energy of every individual spin must be taken into account,

$$\mathcal{H} = -\sum_{(i,j)} \mathbf{J}_{ij}\mathbf{S}_i \cdot \mathbf{S}_j + \sum_i U_i S_i^z. \tag{5.11}$$

One reasonable and common assumption is that the exchange interaction has a very short range of action, so that $\mathbf{J}_{ij}$ is usually considered to be zero when i and j are not nearest neighbours and constant when they are, $\mathbf{J} = (J^x, J^y, J^z)'$, in particular if there are periodic boundary conditions and the atoms are identical. U_i is also usually considered to be constant.

In order to get a better intuition for the behaviour of chains governed by this Hamiltonian, let us look at some very simple cases. One of the simplifications we will assume is $J^x = J^y = 2J_\perp$ (the XXZ model), which allows the Hamiltonian to be written in terms of spin-flip operators. In a straight chain with open boundary conditions,

$$\begin{aligned}\mathcal{H} &= 2J_\perp \sum_{i=1}^{N-1} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right) + J_z \sum_{i=1}^{N-1} S_i^z S_{i+1}^z + U \sum_{i=1}^{N} S_i^z \\ &= J_\perp \sum_{i=1}^{N-1} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + J_z \sum_{i=1}^{N-1} S_i^z S_{i+1}^z + U \sum_{i=1}^{N} S_i^z . \end{aligned} \tag{5.12}$$

5.3.1 Relation to Hubbard model

One may legitimately ask now what kind of systems are modelled by the Heisenberg Hamiltonian and what is its physical meaning. To answer this question, even in a qualitative way, we have to look at a very simple model of systems that exists in Nature, the Hubbard model, which has been said to be "both the best studied and the least understood in magnetism" (7). The model assumes that (1) electrons may hop from one site to its nearest neighbour with energy gain t because molecular orbitals, where electronic wave functions are spread across several atoms, are in general less energetic than atomic orbitals, (2) it is hard for two electrons to be at the same site due to Coulomb repulsion energy U and (3) Pauli's exclusion principle holds. Accordingly, the Hubbard Hamiltonian is given by

$$\mathcal{H}_{Hubb} = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}\right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} . \tag{5.13}$$

Here $\langle i, j \rangle$ denotes nearest neighbours i and j, and $c_{i,\sigma}^\dagger$, $c_{i,\sigma}$ and $n_{i,\sigma}$ are the fermionic creation, annihilation and number of occupation operators for site i and spin z-component σ.

Long distance interactions as well as higher energy levels are not considered in this model, which is a fair approximation for electrons in a periodic potential such as a lattice or chain at low temperature. In the low energy, half-filling situation, when $\langle n \rangle = 1$, perturbation theory may be applied to this Hamiltonian, allowing it to be re-written as a Heisenberg Hamiltonian (7).

This equivalence between the two models in restricted conditions indicates the origin of the exchange interaction between spins: it is not related to the direct interaction between the spin angular momenta of electrons, too faint to be considered in the Hubbard model, but rather to the familiar Coulomb repulsion between them which, due to the Pauli exclusion principle, causes certain spin configurations to be preferred over others.

5.3.2 Isotropic Heisenberg Model

We will now look at some more limiting cases of the Heisenberg model so that we may get an intuition for its general behaviour. Let us start by considering the simple case of a chain with N spins with no magnetic field, $U = 0$, and isotropic $J > 0$. The so-called isotropic ferromagnetic Heisenberg Hamiltonian is then

$$\mathcal{H}_{iso} = -J \sum_{i=1}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \tag{5.14}$$

A ground state of this Hamiltonian is the one where all spins are aligned in the positive direction of the z-axis, $|\phi\rangle = |\uparrow\uparrow\uparrow \ldots \uparrow\rangle$, since each of the $N-1$ pairs of nearest neighbours forms a triplet:

$$\mathcal{H}_{iso}|\phi\rangle = -\frac{1}{4}(N-1)J|\phi\rangle.$$

Now we analyse what happens to a small perturbation of the ground state, a single flipped spin that is called a *magnon*. The simplest case is that in which the perturbation is localised in a single site, at position j (we will assume that the perturbation is somewhere in the middle of the chain, this is, $j \neq 1, N$). The perturbed state may be written as $|j\rangle = S_j^- |\phi\rangle$ and is not an eigenstate of the Hamiltonian,

$$\begin{aligned}
\mathcal{H}_{iso}|j\rangle &= -J\left(\sum_{i\neq j-1,j}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}.\right)|j\rangle - J\left(\mathbf{S}_{j-1}\cdot\mathbf{S}_j.\right)|j\rangle - J\left(\mathbf{S}_j\cdot\mathbf{S}_{j+1}.\right)|j\rangle \\
&= -\frac{1}{4}(N-3)J|j\rangle - \frac{1}{2}J|j-1\rangle + \frac{1}{4}J|j\rangle - \frac{1}{2}J|j+1\rangle + \frac{1}{4}J|j\rangle \\
&= -\frac{1}{2}J|j-1\rangle - \frac{1}{4}(N-5)J|j\rangle - \frac{1}{2}J|j+1\rangle.
\end{aligned}$$

Once again we may see a trend to scatter the perturbation through the chain. In fact, this Hamiltonian is equivalent to a tight-binding model (the limit case of the Hubbard model in which $U = 0$, i.e., the only term is due to the hopping of particles) with an extra diagonal term and has eigenstates in which perturbations, even if only a single one, are delocalised across all the sites,

$$|q\rangle = \sqrt{\frac{2}{N+1}} \sum_j \sin\left(\frac{qj\pi}{N+1}\right)|j\rangle, \tag{5.15}$$

There are two lessons to retain from this simple example: the first one is that the S^z term of the Hamiltonian is *static*, in the sense that it does not change the position of the flipped spin but rather assigns it a value of energy $\pm J_z$ ($S_i^z S_{i+1}^z|j\rangle = \pm 1/4|j\rangle$), while the S^x and S^y (or S^+ and S^-) term has a *kinetic* role, propagating perturbations through the chain.

The second lesson is that in the absence of a magnetic field the isotropic ferromagnetic Heisenberg model favours ordered spins and very delocalised perturbations: an initial product state with a single localised perturbation $|j\rangle$, in which any subsystem formed by a single qubit is pure, will quickly evolve towards a superposition of states in which all subsystems are mixed. This way, the entropy of single qubits in the chain is expected to increase rapidly under time evolution.

5.3.3 Other limits

In the Ising limit, $J_x = J_y = U = 0$, there is no magnetic field and no "kinetic" term,

$$\mathcal{H}_{Ising} = -J_z \sum_{i}^{N-1} S_i^z S_{i+1}^z. \tag{5.16}$$

This model is purely static and any configuration of spins up and down along the z-direction is an eigenstate. If $J_z > 0$ ferromagnetic configurations are favoured and vice versa. The opposite limit, where $J_z = U = 0$, is called the XY model and is described by the Hamiltonian

$$\mathcal{H}_{XY} = \sum_{i}^{N-1} J_i \left(S_i^+ S_{i+1}^- + S_i^+ S_{i+1}^- \right). \tag{5.17}$$

In this case the chain exhibits an extremely dynamic behaviour. Any perturbation is propagated as fast as the coefficients are large and for the certain values of J_i's it is even possible to achieve perfect state transfer – the reproduction, after some time, of a state that was originally at the beginning of the chain at its end (2). This phenomenon has important applications in quantum communications.

In this work we will study the XXZ limit,

$$\mathcal{H}_{XXZ} = J_\perp \sum_{i=1}^{N-1} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) + J_z \sum_{i=1}^{N-1} S_i^z S_{i+1}^z, \tag{5.18}$$

wherein $J_z \gg J_\perp \neq 0$. This is a mainly static model that allows slow propagation of antiferromagnetic perturbations.

Chapter 6

Numerical simulations

We performed a series of numerical simulations in spin chains in order to test the evolution of quantum entropy measures as subsystems of the chains thermalised. In this chapter we present the goals, technical specifications and main results of these simulations.

6.1 Goals

We used the spin chains as toy systems to study the behaviour of entropy measures in small quantum systems and the thermalisation process of such systems. With the simulations we expected to obtain an intuition to the answers of some concrete questions:

1. How does the thermalisation process depend on the initial state of the total system?

2. How small compared to the rest of the system must a subsystem be in order to equilibrate?

3. Small quantum systems have a marked periodic behaviour. Even so, do subsystems inside such systems spend most of the time close to an equilibrium state?

4. The max-entropy only takes a few possible values for small quantum states. Do the Rényi entropies of order $\alpha < 1$ follow this discrete behaviour?

5. Similarly, is the time evolution of Rényi entropies of order $\alpha > 1$ similar to that of the min-entropy for really small systems?

6. Does entropy saturate as the subsystem reaches equilibrium? Does the equilibration time determine the saturation time of all entropy measures or do some of them saturate before that?

7. Do the answers to these questions provide criteria that can help to decide which entropy measures, if any, better characterise the state and evolution of very small quantum systems?

6.2 About the simulations

We studied spin chains of 3 to 10 qubits evolving under a XXZ Hamiltonian to which a small *noise* term was added:

$$\mathcal{H}_{XXZ} = J_\perp \sum_{i=1}^{N-1} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) + J_z \sum_{i=1}^{N-1} S_i^z S_{i+1}^z + \delta R, \tag{6.1}$$

where $J_z \gg J_\perp \gg \delta$ and R is a Hermitian random matrix of norm $||R||_\infty \approx 1$. Unless stated otherwise, the values used in the simulations were $J_z = 100.0$, $J_\perp = 2.0$ and $\delta = 0.01$, in units of $\hbar$.

The random term ensures that the Hamiltonian does not have degenerate energy gaps and increases the effective size of the basis of the system by inducing transitions between subspaces of different total magnetisation, which are not allowed by the non-noisy XXZ model. The noise has a very natural physical interpretation – it may be seen as a weak coupling interaction that exists in nature and is ignored by the Heisenberg model, as well as a perturbation caused by small imperfections in the lattice (4).

The initial state of the spin chain is taken to be pure and product in the canonical basis. This way the initial state is also pure for a small subsystem of interest, composed of one or two qubits near the centre or one of the extremities of the chain.

As the spin chain evolved under the action of the Hamiltonian of Eq. 6.1, some properties of the subsystem were evaluated. First, to get an idea of the periodicity of the time evolution of the chain, we studied the distance of the subsystem to its initial state. If the subsystem gets very close to its original state that indicates that the same has probably happened with the global system.

Then we studied the equilibration of the subsystem. We obtained the time-average state of the subsystem by summing the reduced density matrices of 200 000 instants chosen at random over a long period of time, and then computed the distance between the state of the subsystem at a given time and this average state. In the cases where this distance was small most of the time we could conclude that the subsystem had equilibrated and that the average reduced density matrix represented the equilibrium state.

Finally we evaluated several entropy measures over time: the min-, smooth min- (with $\varepsilon = 0.05$ unless stated otherwise) and $\alpha = 2$ Rényi entropies, the von Neumann entropy and the max-, smooth max- and $\alpha = \frac{1}{2}$ Rényi entropies, all of them applied to the subsystem.

Here we present the main results for chains of 3 to 7 qubits. The simulations were programed in *Mathematica 7.0* ©. The code may be found in the appendix.

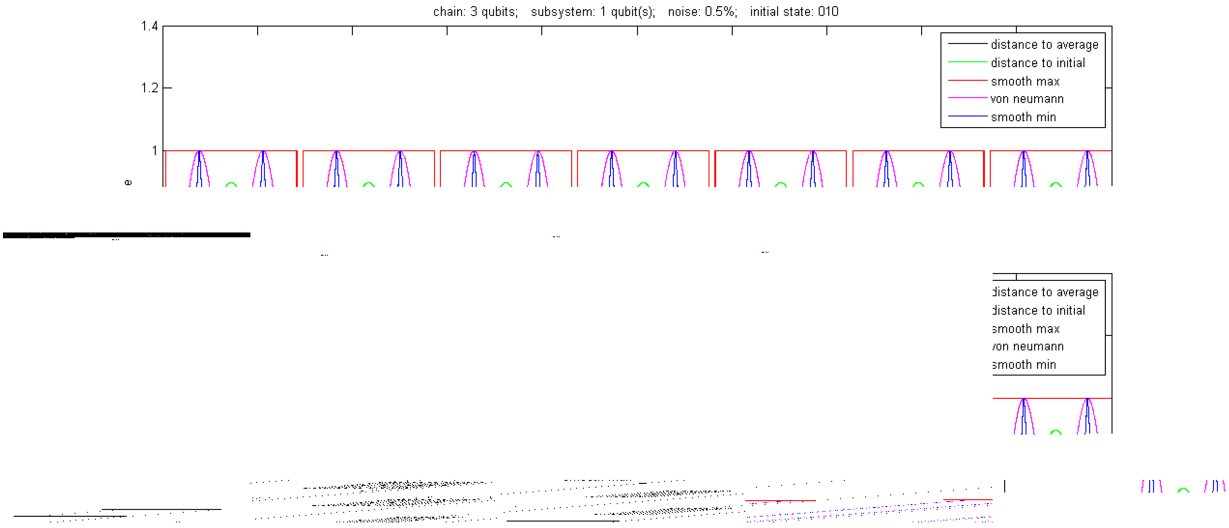


Figure 6.1: Three-qubit spin chain. Subsystem with one qubit. Time evolution of the main quantum entropy measures and of the distance to initial and average states. Simulation parameters: $\varepsilon = 0.005$, $\Delta t = 0.01$, $T = 2000$, 200000 steps.

6.2.1 Technical drawbacks

The exponential increase of the size of the basis with the number of qubits made it impossible to simulate accurately larger spin chains in a reasonable time.

Numerical errors led in two cases to an imaginary term of order $\approx 10^{-8}$ in von Neumann and $\alpha = \frac{1}{2}$ Rényi entropies. This term was ignored in the final results.

6.3 3-qubit chain: the simplest case

We started by considering a spin chain with only 3 qubits prepared in the initial state $|\downarrow\uparrow\downarrow\rangle$. The subsystem of interest was the central qubit. We expected a small system like this to have a small period and indeed that may be observed in Fig. 6.1 as the distance to the original state of the subsystem (green in the figure) reaches zero quickly after a maximum value of nearly 0.9. The other quantities follow the periodicity of the distance to the initial state.

We also see in that figure and in Fig. 6.2 that the state becomes fully mixed twice every cycle, with all entropy measures reaching the maximum value of one. Note that the fully mixed state, $\frac{1}{2}(|\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\uparrow|)$, is also the average state.

The max- and smooth max-entropies are of little interest in this case, since they may only take two possible values, 0 and 1, the logarithm of the number of non-zero eigenvalues of the reduced density matrix (with some tolerance in the case of the smooth max-entropy). They saturate extremely fast and almost always coincide. The $\alpha = \frac{1}{2}$ Rényi entropy follows this behaviour in a continuous, smoother way.

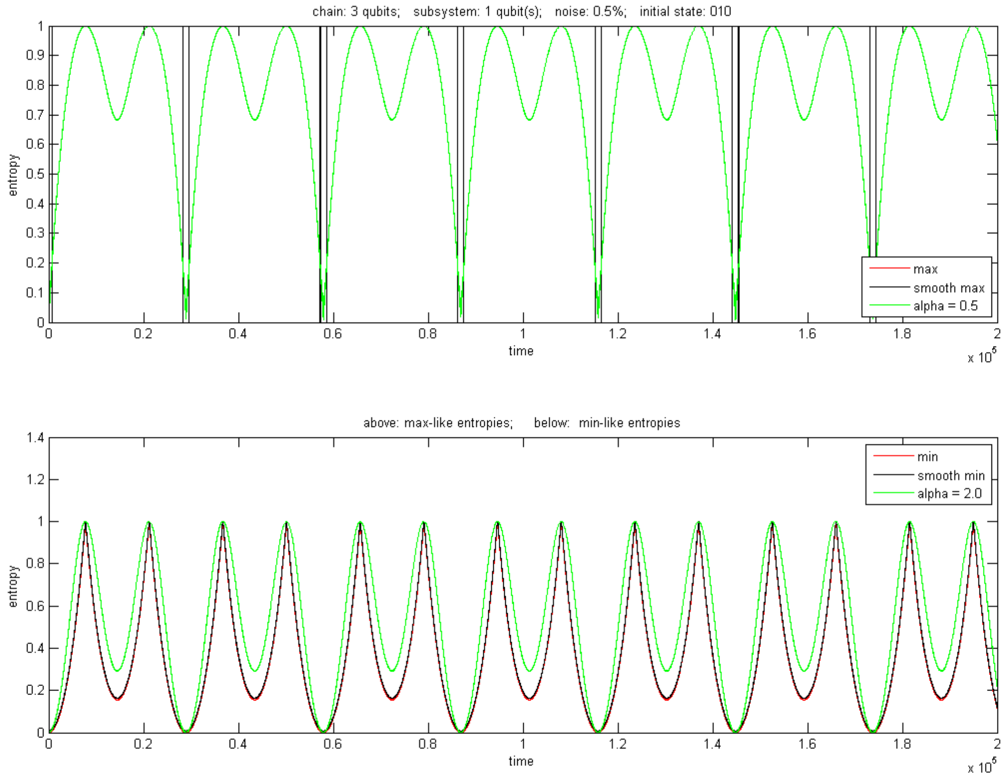


Figure 6.2: Three-qubit spin chain. Subsystem with one qubit. Time evolution of the two families of quantum entropy measures. Simulation parameters: $\varepsilon = 0.005$, $\Delta t = 0.01$, $T = 2000$, 200000 steps.

The min-entropy is followed closely by its smooth version and by the $\alpha = 2$ Rényi entropy. These entropies nearly mirror the behaviour of the distance to the average state. The von Neumann entropy is, as predicted, in between the two main families of Rényi entropies.

6.4 4-qubit chain: the importance of noise

After studying the case $N = 3$ we considered a 4-qubit spin chain when the subsystem of interest is half of the chain and there is no bath in the thermodynamic sense of it, only another subsystem of the same size. In these conditions we tested the importance of the noise term in the Hamiltonian, by comparing simulations with and without noise.

The initial state of the chain was $|\uparrow\uparrow\downarrow\downarrow\rangle$ and we began by considering the subsystem formed by the first two qubits (Fig. 6.3). There is no obvious periodicity in the time interval of the simulation – at most we may say that the subsystem returns to a state

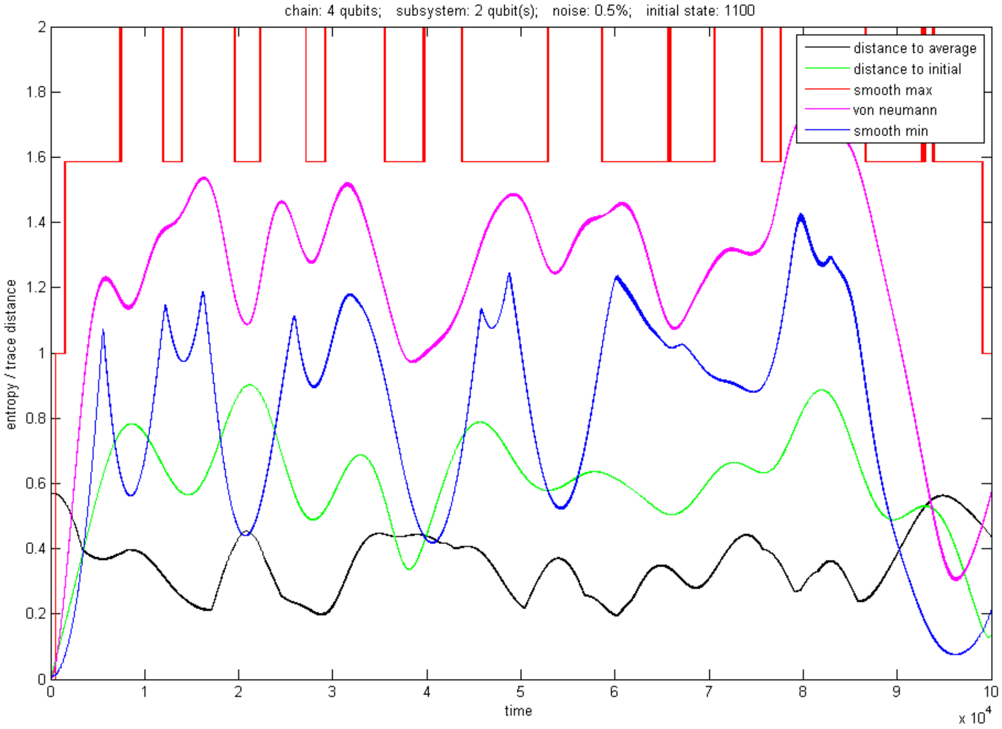


Figure 6.3: Time evolution of the main quantum entropy measures and of the distance to initial and average states of a two-qubit subsystem in a four-qubit spin chain, under the action of a noisy XXZ Hamiltonian. Notice that there no periodicity is apparent here. Simulation parameters: Subsystem formed by the first two qubits. Initial state with the qubits of the subsystem excited: $|\uparrow\uparrow\downarrow\downarrow\rangle$. $\varepsilon = 0.005$, $\Delta t = 0.01$, $T = 1000$, 100000 steps.

close to the initial one near the end of the time of study.

However, as we repeated the simulation (for the same time interval) without the small random perturbation of the Hamiltonian, the subsystem presented a marked periodic behaviour (Fig. 6.4), reflecting the smaller number of states that it may go through.

The entropy measures of the two-qubit subsystem showed the same periodicity. The behaviour of some of the entropy measures during the first two periods is depicted in Fig. 6.5. The three Rényi entropies of order greater than one (min-entropy, smooth min-entropy and $\alpha = 2$ Rényi entropy) display the same periodic behaviour, although they are considerably different in value. All the plots give the illusion of a superposition of continuous curves but they are extremely discontinuous with the value of the entropy shifting from one of the apparent curves to another in every time step. This indicates an extremely fast, periodic variation of the quantities observed, a variation whose amplitude is modulated by an envelope function that has a much larger period.

The max- and smooth max-entropy saturated rapidly and remained constant almost

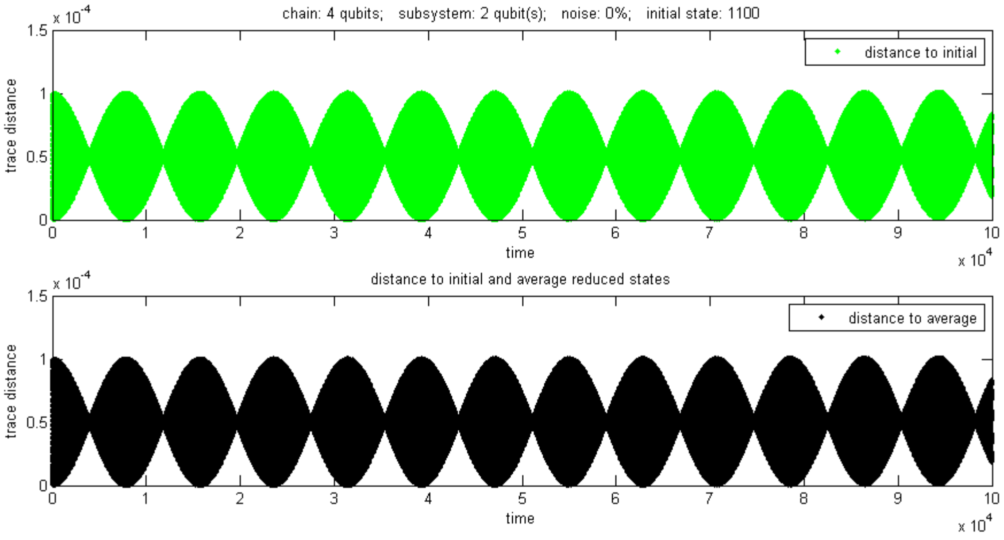


Figure 6.4: Time evolution of the of the distance to initial and average states of a two-qubit subsystem in a four-qubit spin chain, under the action of a pure XXZ Hamiltonian. The system shows a marked periodicity, returning to the initial state very quickly when compared to the noisy case. Simulation parameters: Subsystem formed by the first two qubits. Initial state with the first two qubits excited: $|\uparrow\uparrow\downarrow\downarrow\rangle$. $\varepsilon = 0.005$, $\Delta t = 0.01$, $T = 1000$, 100000 steps.

all of the time, like in the case of a chain with 3 qubits. The Rényi entropy of order 0.5 has values close to those of the smooth max-entropy, as expected, but its behaviour is very different from the flat one exhibited of the max-entropies. In fact, it does not even follow the simple periodicity of the min-entropies, as shown in Fig. 6.5 (pink curve).

We obtained the same periodic behaviour when studying the subsystem formed by the two qubits of the middle of the chain, under the same conditions (Fig. 6.6).

6.5 6-qubit chain: emergence of equilibration

In order to increase the period of the oscillations observed in the evolution of entropies and achieve thermalisation, larger global systems must be considered. The first signs of equilibration were observed as we analysed a two-qubit subsystem inside an six-qubit spin chain. The chain was initialised in state $|\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\rangle$.

Fig. 6.7 depicts the increase and saturation of the main entropy measures as the subsystem diverts from its initial state and approaches the average state. The rest of the entropies are represented in Fig. 6.8 . No periodicity was apparent in the time interval studied, a result of the already reasonable size of the system, induced by both a higher number of qubits and the presence of noise in the XXZ Hamiltonian. Like in the previous cases the max-entropies saturated much faster than all the other quanti-

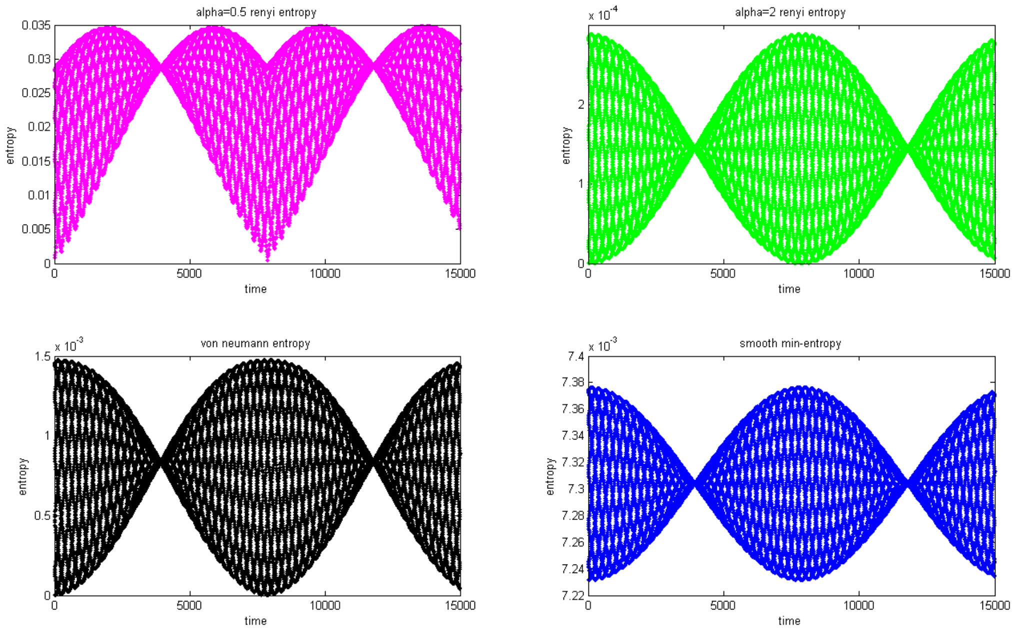


Figure 6.5: Zooming in on some entropy measures of a four-qubit spin chain with a subsystem formed by the first two qubits that evolve under the action of a pure XXZ Hamiltonian. The quantities change quickly as a fast periodic function modulated by a much slower envelope function and thus giving the illusion of many continuous curves. Simulation parameters: Initial state with the first two qubits excited: $|\uparrow\uparrow\downarrow\downarrow\rangle$. $\varepsilon = 0.005$, $\Delta t = 0.01$, $T = 1000$, 100000 steps.

ties observed. The min- and smooth min-entropies evolved more slowly than the other entropy measures but, just like the others, increased approximately linearly in the beginning of the simulation and then remained close to an average value of, in this case, 1. This behaviour – a quick, pseudo-linear saturation followed by a long period of small oscillations around a mean value – is typical of a thermalising system.

We do not consider the average state an equilibrium state based on this data since in the time window studied the subsystem never reached the close proximity of that state: $\delta(\rho_S(t), \langle\rho_S\rangle) > 0.1$ for all t observed. A larger system would be necessary to increase the proximity to equilibrium.

Tests with different initial states showed similar quasi-equilibration behaviour results. However, the average state of both the global system and the subsystem depended on the initial state of the system, even for states with the same total magnetisation, for instance two magnons in different initial positions.

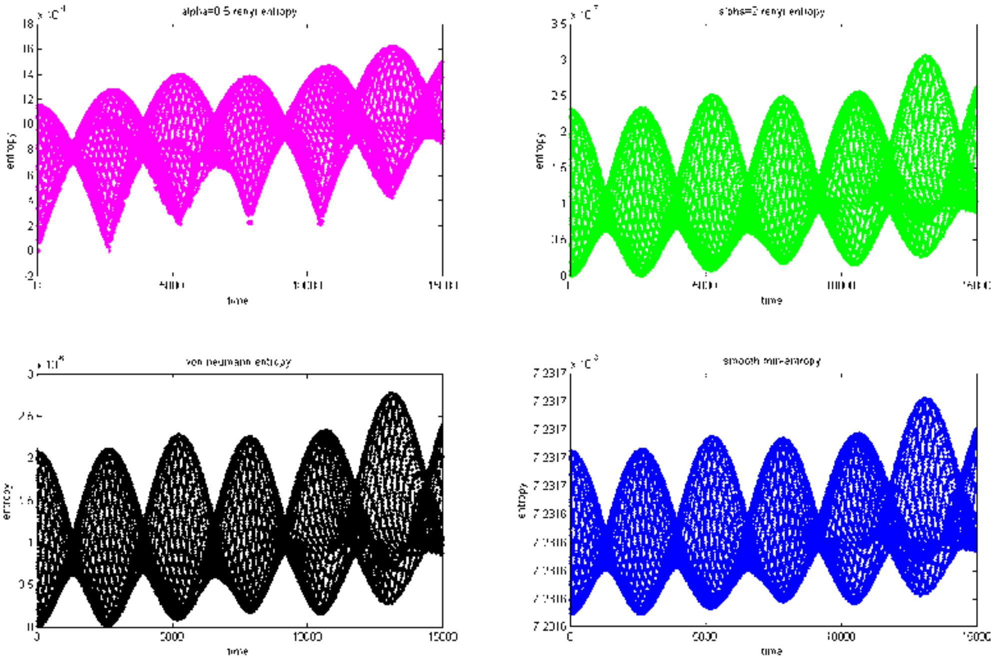


Figure 6.6: Zooming in on some entropy measures of a four-qubit spin chain with a subsystem formed by the central two qubits that evolve under the action of a pure XXZ Hamiltonian. Again the quantities change quickly and are modulated by a much slower envelope function, that is slightly different that in the previous case, since the subsystem of study has different properties (namely is not in the extremity of the chain). Simulation parameters: Initial state with the first two qubits excited: $|\uparrow\uparrow\downarrow\downarrow\rangle$. $\varepsilon = 0.005$, $\Delta t = 0.01$, $T = 1000$, 100000 steps.

6.6 7-qubit chain: a magnon

The results presented in chapter four indicate that the relation between the (effective) dimensions of subsystem and bath is the main criterion to achieve thermalisation. Considering this, we studied a subsystem of a single qubit in a seven-qubit spin chain prepared in the state $|\downarrow\downarrow\downarrow\uparrow\downarrow\downarrow\downarrow\rangle$. Our subsystem is a magnon in an originally ferromagnetic chain. We compare the results of simulating this system with and without the noise term in the Hamiltonian.

When there is no noise (Fig. 6.9) the distance to initial and average states show, like in the four-qubit chain, a periodic fast behaviour modulated by a periodic envelope function. The subsystem returns to the initial state after a while – even the smooth max-entropy reaches zero at that point, as may be seen in Fig. 6.10. The exact behaviour of the von Neumann remains unclear as the time step is too big to give a good idea of the time variation of the enveloped function, but it is obvious that the envelope is also

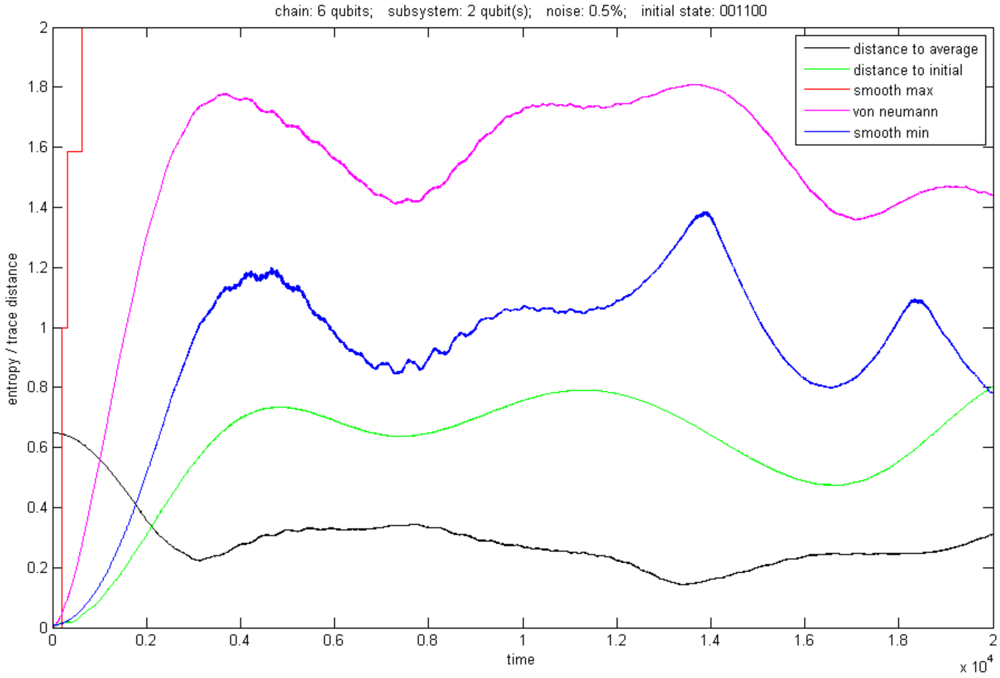


Figure 6.7: Approximate equilibration of a two-qubit subsystem in a six-qubit chain: time evolution of the main quantum entropy measures and of the distance to initial and average states. The entropy measures increase linearly, saturate and then oscillate non-periodically around a certain value. Observe that max- and von Neumann entropy saturate faster than the distance to average state. The min-entropy, on the other hand, saturates approximately at the same time than this distance and thus is a good indicator of whether the subsystem has termalised. Simulation properties: Subsystem formed by the two central qubits. Initial state with the qubits of the subsystem excited: $|\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\rangle$. $\varepsilon = 0.005$, $\Delta t = 0.01$, $T = 200$, 20000 steps.

periodic.

It is interesting to observe the way that the introduction of noise breaks the periodicity of the behaviour of the quantities tested - see Fig. **??**. Since the dimension of the total system is much larger than in the case of a chain of only four qubits, the relative importance of the noise is smaller and the low level of noised that was added to the Hamiltonian is not enough to shut the fast variation of the enveloped functions but clearly destroyed the periodicity of the envelope ones. These are collapsing in a non-periodical way (in particular, the subsystem does not return to its initial state in the time window considered) and the plots would eventually become single lines like those of the six-qubit spin chains if the noise kept increasing. We could then observe equilibration of the magnon.

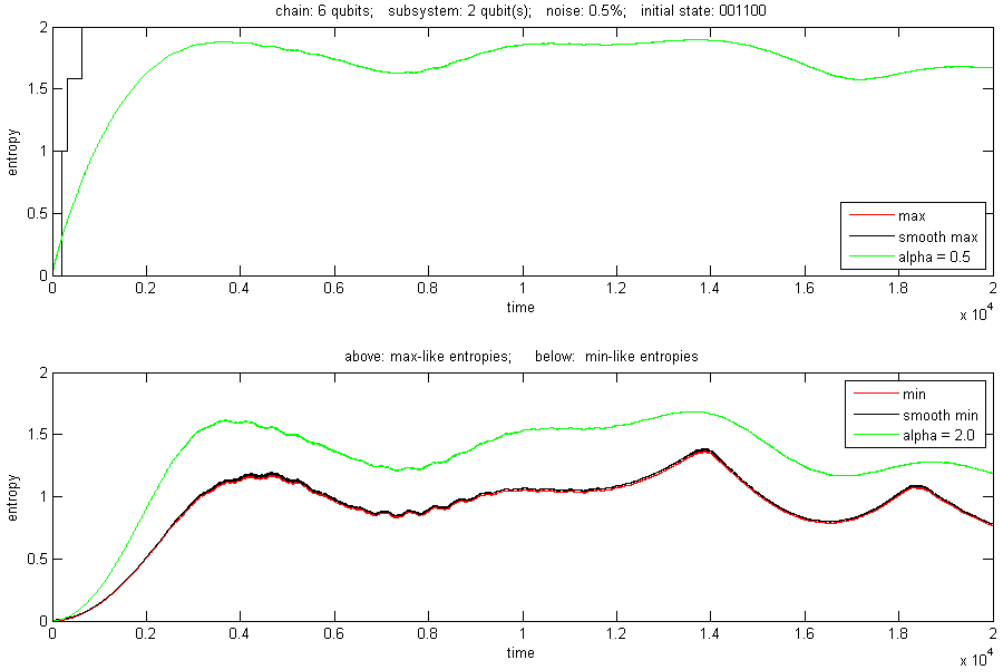


Figure 6.8: Approximate equilibration of a two-qubit subsystem in a six-qubit chain: time evolution of the two families of quantum entropy measures. Simulation parameters: Subsystem formed by the two middle qubits. Initial state with only the qubits of the subsystem excited: $|\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\rangle$. $\varepsilon = 0.005$, $\Delta t = 0.01$, $T = 200$, 20000 steps.

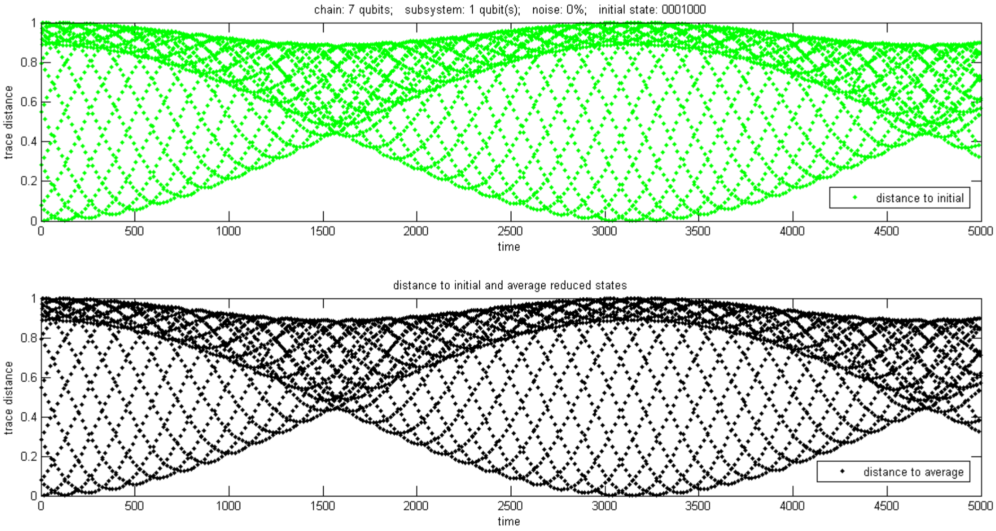


Figure 6.9: Time evolution of the distance to initial and average states of a magnon in a seven-qubit spin chain evolving under a pure XXZ Hamiltonian. Double periodicity of envelope and enveloped functions is present. Simulation parameters: Subsystem formed by the central qubit, initially excited (a magnon). Initial state: $|\downarrow\downarrow\downarrow\uparrow\downarrow\downarrow\downarrow\rangle$. $\varepsilon = 0.005$, $\Delta t = 10$, $T = 1000000$, 100000 steps.

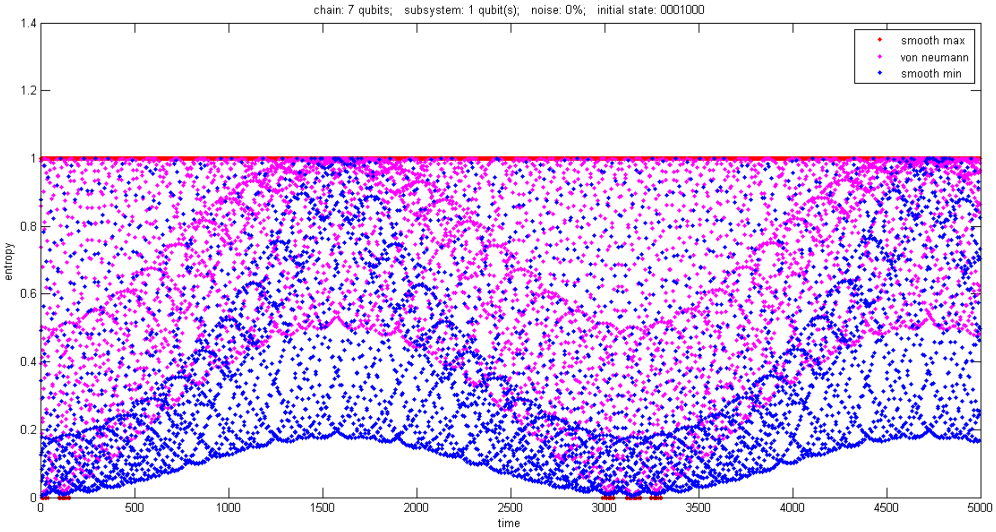


Figure 6.10: Time evolution of the main quantum entropy measures of a magnon in a seven-qubit spin chain evolving under a pure XXZ Hamiltonian. A low periodicity may be observed. Simulation parameters: Subsystem formed by the central qubit, initially excited. Initial state: $|\downarrow\downarrow\downarrow\uparrow\downarrow\downarrow\downarrow\rangle$. $\varepsilon = 0.005$, $\Delta t = 10$, $T = 1000000$, 100000 steps.

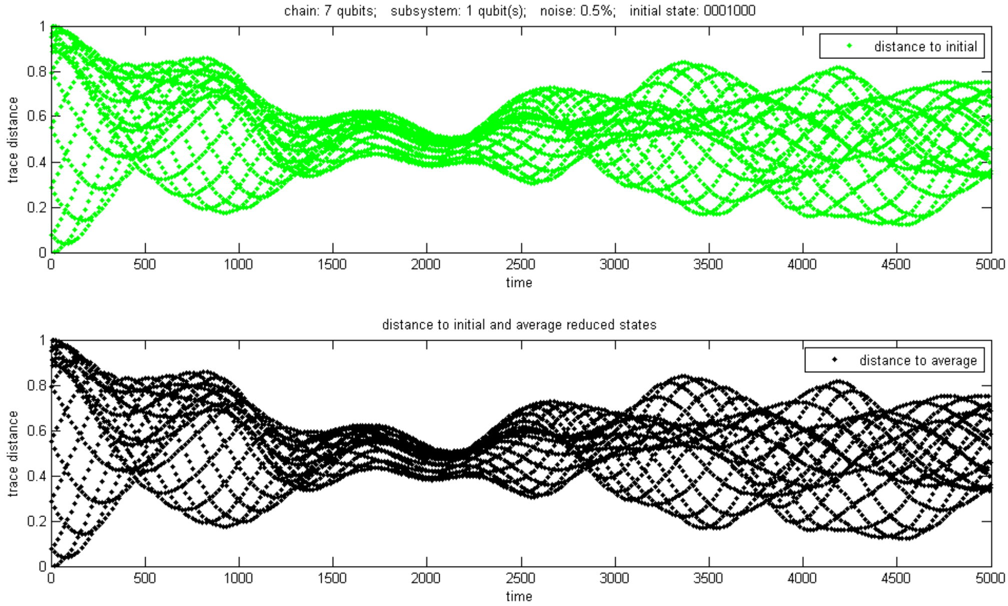


Figure 6.11: Breakdown of periodicity with the introduction of a low level of noise in the Hamiltonian. Simulation parameters: Seven-qubit spin chain. Subsystem formed by the central qubit, initially excited (a magnon). Initial state: $|{\downarrow\downarrow\downarrow\uparrow\downarrow\downarrow\downarrow}\rangle$. Time evolution of the distance to initial and average states. $\varepsilon = 0.005$, $\Delta t = 10$, $T = 1000000$, 100000 steps.

Chapter 7

Conclusions and future work

The goal of this project was to study the behaviour of quantum entropy measures in small quantum systems, in order to get an intuition for the subject that could help to orientate a future project dedicated to the development of a thermodynamic theory of small quantum systems based on quantum entropies.

We have seen how to model composite (in particular interacting) quantum systems. We introduced the notion of quantum entropy and discussed the physical meaning of some entropy measures and the relations between them. We presented a quantum-information framework to the phenomena of thermalisation and equilibration and recalled state-of-the-art results in this topic. Then we introduced the toy systems of study, Heisenberg spin chains, from the most basic principles of spin and exchange interaction. We discussed their physical meaning and how they behaved under the action of the XXZ Hamiltonian. To contribute to that body of work we finally developed and performed numerical simulations in those spin chains in order to study the behaviour of several entropy measures as small systems thermalised.

The analysis of the results of simulations have helped us to better understand the behaviour of small quantum systems and of the entropy measures. Below is a summary of some of the more relevant observations:

1. We have seen (for instance for six-qubit chains) that different initial states of the global system cause differences in the average states of system and subsystem. This was the case even if the initial states had the same macroscopic parameters (in this case the total magnetisation).

2. We started by testing a three-qubit chain and increased the size of the chain gradually. The first signs of equilibration were observed in a two-qubit subsystem in a six-qubit chain. In the case of a one-qubit subsystem in a seven-qubit chain we have seen that as a noise term was added to the XXZ Hamiltonian the periodicity of the behaviour of the subsystem was partially broken. One of the reasons for this phenomenon is the fact that the noise term greatly increases the effective dimension of the system. Another is that the noise term introduces interactions between all qubits – in a sense the subsystem is in contact with all the system and

not only with the two next neighbours. This makes propagation of perturbations and consequent equilibration become much more intensive.

3. The trace distance between the state of the subsystems at a given time and the "equilibrium" state was in (time) average equal or greater than 0.2 for all the systems studied. In these conditions we cannot say that any of the states has fully equilibrated. We could probably observe equilibration for slightly larger systems – but those are too heavy for the computational and time resources available for this project.

4. We have seen that the Rényi entropy $H_{0.5}$ followed the behaviour of the max-entropies but in a continuous way – which often led to plots noticeably different from the stepped ones that represented the max-entropy. We expect that for larger systems, as the max-entropies may take more (and closer) possible discrete values and the smooth max-entropy diverges from the non-smooth version, the $H_{0.5}$ entropy will start to resemble the smooth max-entropy more.

5. In the same way the Rényi entropy of order two had a behaviour very similar to that of the smooth min-entropy, although in some concrete cases it had much higher values.

6. In the cases where some equilibration process was observed, all the entropy measures exhibited an initial pseudo-linear rapid increase followed by a kind of saturation behaviour of non-harmonic oscillations around a saturation value (although only the max-entropies reached their maximum possible value). This behaviour resembles the second law of thermodynamics.

7. The max-entropies saturated much faster than the min-entropies. Indeed, the max-entropies saturated at their maximum value for almost all times in all the cases studied, even those with a marked periodical behaviour. At least for the very small subsystems that we have seen here, max-entropies are not good indicators of whether a subsystem has thermalised or not, since they saturate much faster than the distance to the average state.

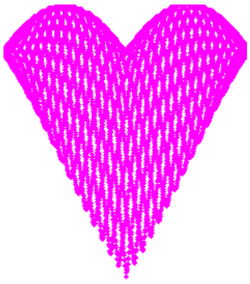
8. The min-entropies, on the other hand, saturated much slower – in fact they only stabilised as the distance to the average state did the same. In general, these entropies had a stable behaviour when the subsystem was close to the average state. They seem to have potential to be used as evidence about the equilibration state of a subsystem.

9. There was nothing especially remarkable about the von Neumann entropy, which was always a middle term between H_2 and $H_{0.5}$ (and therefore with values between min- and max-entropy). This is consistent with our interpretation of the von Neumann entropy as a mean entropy.

We did not have the opportunity to study deeply, from an analytical point of view, the results presented in chapter four, leaving some open questions for a future, longer project about the relation between entropy measures and thermalisation of general quantum systems.

On the other hand, after analysing the numerical results obtained in this project, some new questions were raised, questions that may be answered either with more numerical work or with a theoretical approach. Some of the question that motivate future work on the topic are:

1. Are the bounds presented in chapter four tight for slightly larger systems? Can we improve those bounds using for instance the smooth min-entropy instead of the Rényi entropy of order two?
2. Does the smooth max-entropy become a more interesting and relevant quantity for subsystems that are much larger than the ones tested but still too small for the classical thermodynamic limit (for instance, subsystems with a hundred qubits)?
3. In general, do our conclusions hold as the toy systems (spin chains) scale up?
4. Do our conclusions hold for other kind of toy systems? Is the thermalisation process very different in, for instance, 2D and 3D lattices? And in gases, liquids and glasses?
5. The (smooth) min-entropy seems a good candidate for becoming the *standard* entropy of a thermodynamics of small systems. Is it possible to derive other useful and thermodynamics-related quantities, such as temperature, from this entropy?
6. Do small quantum systems thermalise in the Boltzmannian form $\boldsymbol{\rho}_S^{\mathbf{eq}} = \frac{\exp(-H_S\beta)}{Z}$? Is it possible to obtain a temperature measure adequate for small systems from the analysis of equilibrated quantum states of this form?



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Appendix

Here we present the code for the numerical simulations, which were programmed in *Mathematica 7.0* ©. We may provide the original file by request. Our contact email is lidia.del.rio@ua.pt . We are Lídia del Rio.

We would like use the rest of this page to thank Oscar for all his support.

Thank you Oscar!

Thank you Oscar!

Thank you Oscar!

Thank you Oscar!

Thank you Oscar!

Thank you Oscar!

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Thank you Oscar!

XZ model + noise in a spin chain and entropy measures

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Late first steps for my master project: studying the xz model in a spin chain and see how several entropy measures behave in this system.

```
Clear["Global`*"]

startingTime = DateString[]

Sun 5 Jul 2009 03:20:19
```

Functions

Basic functions

Quantum Information stuff

Partial trace

Still needs some optimization.

```
PartialTrace = Function[{matrix, basis, minisystem},
   (*we want to trace out the system except for the qubits that belong to minisystem*)
   (*let's call  bath to the rest*)
   Module[
    {reducedbasis,
     reducedmatrix,
     basisi, basisj,
     m, n,
     toskip,
     subsystem,
     test,
```

```
     currentSizeBasis,
     sizeSubsystem},

    (*initial reduced matrix and basis*)
    sizeSubsystem = Length[minisystem];
    reducedmatrix = ConstantArray[0, {2^sizeSubsystem, 2^sizeSubsystem}];
    (*this might be too big, but we will cut the excess at the end*)
    reducedbasis = ConstantArray[ConstantArray[0, sizeSubsystem], 2^sizeSubsystem];
    currentSizeBasis = 0;

    subsystem = Flatten[minisystem]; (*just to make sure this is not a nested list*)
    toskip = Partition[subsystem, 1];
    (*then we need a nested list, that will be useful for the Deletes*)

    Do[

     basisi = basis[[i]];
     basisj = basis[[j]];

     If[
      (*Checks if this is an element of the trace*)
      (*this is,
      if the basis element of the bath is  the same for the line and the column*)
      Delete[basisi, toskip]  == Delete[basisj, toskip] ,

      (* verifies if there is an element of the
        reduced basis of the form of the basis element of the minisystem,
      for the line and for the column. if not, adds it to the reduced basis.*)
      {reducedbasis, m, currentSizeBasis} = SeekOrAdd[reducedbasis,
        basisi[[subsystem]], currentSizeBasis];
      {reducedbasis, n, currentSizeBasis} = SeekOrAdd[reducedbasis,
        basisj[[subsystem]], currentSizeBasis];

      (*if everything is ok,
      sums the element of the matrix to the element of the reduced one.*)
      reducedmatrix[[m, n]] = reducedmatrix[[m, n]] + matrix[[i, j]];

     ],
     {i, 1, Length[matrix]},
     {j, 1, Length[matrix]}

    ];

    (*cutting off the excess*)
    (*in general,
    if the subsystem is much smaller than the total system, this won't cut anything*)
```

```
    reducedmatrix = reducedmatrix[[1 ;; currentSizeBasis, 1 ;; currentSizeBasis]];
    reducedbasis = reducedbasis[[1 ;; currentSizeBasis]];
    (*output*)
    {reducedmatrix, reducedbasis}
   ]
  ];
```

- **Trace distance**

```
TraceDistance = Function[
   (*given two density matrices written in the same basis,
   calculates the trace distance between them. yey!*)
   {matrix1, matrix2},
   Module[
    {egvalues},
    egvalues = HandyEgvalues[matrix1 - matrix2];
    0.5 * Total[Abs[egvalues]]
   ]
  ];
```

Operators

Instead of the symbol |...〉, we use the header *z*

- **spin flip operators**

```
FlipUp = Function[
   {k, state},
   If[
    ListQ[state],
    Switch[
     state[[k]],
     1,
     0,
     0,
     ReplacePart[state, k → 1]
    ],
    0
   ]
  ];

FlipDown = Function[
   {k, state},
   If[
    ListQ[state],
    Switch[
     state[[k]],
     0,
     0,
     1,
     ReplacePart[state, k → 0]
    ],
    0
   ]
  ];
```

occupation number operator

```
n = Function[
   { k, spin, state},
   If[
    ListQ[state],
    If[
     state[[k]] == spin,
     state,
     0
    ],
    0
   ]
  ];
```

- **Other useful operators**

- **inner product of states**

```
scalarproduct[a_, 0] := 0

scalarproduct[a_, b_ + c_] := scalarproduct[a, b] + scalarproduct[a, c];
scalarproduct[a_ + b_, c_] := scalarproduct[a, c] + scalarproduct[b, c];

scalarproduct[factor1_. z[arg1_], factor2_. z[arg2_]] :=
 factor1 * factor2 * If[arg1 == arg2, 1, 0]
```

- **sigma bar**

```
Bar = Function[
   spin,
   Mod[spin + 1, 2]
  ];
```

- **z (vacuum condition)**

```
z[0] := 0
```

Entropy Measures (given the eigenvalues)

Given the eigenvalues, these functions calculate the entropy measures.
Since we have to calculate the eigenvalues once, it seems a waste of time to repeat it for every entropy measure.

- **von Neumann entropy**

```
VonNeumannEntropyEg = Function[
   egvalues,
   - Total[
     HandyMultiplication[
      egvalues,
      Log[2, egvalues]
     ]
    ]
  ];
```

Min - entropy

```
MinEntropyEg = Function[
   egvalues,
   -Log[
     2,
     Max[egvalues]
    ]
  ];
```

- ### Max - entropy

```
MaxEntropyEg = Function[
   egvalues,
   Log[
    2,
    Length[egvalues] - Count[egvalues, 0]
   ]
  ];
```

- ### Rényi entropies

```
RenyiEntropyEg[0, egvalues_] := MaxEntropyEg[egvalues];

RenyiEntropyEg[1, egvalues_] := VonNeumannEntropyEg[egvalues];

RenyiEntropyEg[Infinity, egvalues_] := MinEntropyEg[egvalues];

RenyiEntropyEg[alpha_, egvalues_] :=
  (1 - alpha) ^ (-1) *
   Log[
    2,
    Total[
     egvalues ^ alpha
    ]
   ];
```

- ### Smooth max - entropy

```
SmoothMaxEntropyEg = Function[
   {egvalues, epsilon},
   Module[
    {inflated},
    inflated = Crisis[egvalues, epsilon];
    MaxEntropyEg[inflated]
   ]
  ];
```

- ### Smooth min - entropy

```
SmoothMinEntropyEg = Function[
   {egvalues, epsilon},
   Module[
    { flattened},
    flattened = Flattening[egvalues, epsilon];
    MinEntropyEg[ flattened ]
   ]
  ];
```

Entropy measures (given the density matrix)

- ### von Neumann entropy

```
VonNeumannEntropy = Function[
   {matrix},
   Module[
    {eigenvalues},
    eigenvalues = HandyEgvalues[matrix] ;
    VonNeumannEntropyEg[eigenvalues]
   ]
  ];
```

- ### Min - entropy

```
MinEntropy = Function[
   matrix,
   Module[
    {eigenvalues},
    eigenvalues = HandyEgvalues[matrix] ;
    MinEntropyEg[eigenvalues]
   ]
  ];
```

- ### Max - entropy

```
MaxEntropy = Function[
   matrix,
   Module[
    {eigenvalues},
    eigenvalues = HandyEgvalues[matrix] ;
    MaxEntropyEg[eigenvalues]
   ]
  ];
```

- **Rényi entropies**

```
RenyiEntropy[alpha_, matrix_] :=
  Module[
   {eigenvalues},
   eigenvalues = HandyEgvalues[matrix] ;
   RenyiEntropyEg[alpha, eigenvalues]
  ];
```

- **Smooth max - entropy**

```
SmoothMaxEntropy = Function[
   {matrix, epsilon},
   Module[
    {eigenvalues},
    eigenvalues = HandyEgvalues[matrix] ;
    SmoothMaxEntropyEg[eigenvalues, epsilon]
   ]
  ];
```

- **Smooth min - entropy**

```
SmoothMinEntropy = Function[
   {matrix, epsilon},
   Module[
    {eigenvalues},
    eigenvalues = HandyEgvalues[matrix] ;
    SmoothMinEntropyEg[eigenvalues, epsilon]
   ]
  ];
```

Reduced density matrices

- **Tracing over subsystems to obtain reduced basis and density matrices**

```
ReducedSystem = Function[
   {densityCanTotal, systemBasis, sitesChain, sitesSubsystem, position},
   Module[
    {initialPosition},
    initialPosition = 1 + position * Floor[sitesChain / 2 - sitesSubsystem / 2];
    PartialTrace[
     densityCanTotal,
     systemBasis,
     Table[{i} , {i, initialPosition, initialPosition + sitesSubsystem - 1}]
    ]
   ]
  ];
```

```
ExcitedSubsystem = Function[
   {sitesChain, sitesSubsystem, position},
   Module[
    {initialPosition, finalPosition},
    initialPosition = 1 + position * Floor[sitesChain / 2 - sitesSubsystem / 2];
    finalPosition = initialPosition + sitesSubsystem - 1;
    PadRight[ PadLeft[ConstantArray[1, sitesSubsystem], finalPosition], sitesChain]
   ]
  ];
```

XZ Model

Size of chain

We start from a spin chain of size "sites".

For now we assume that in there is exactly one fermion with spin up or down on each site : no double occupancies and no vacancies.

The number of spin - up and spin - down fermions is free.

Spins up will be represented by 1's, while spins down will be 0's.

```
sites = Input[" Total number of qubits: "]
```

```
3
```

```
numberStates = 2^sites
```

```
8
```

```
statesBasis = Table[Num2bits[i, sites], {i, numberStates}];
```

The number of spins up and down may now change, due to the noise term in the Hamiltonian

```
numberSpinsUp = Input["Initial number of spins up: "]
```

```
1
```

- **To noise or not to noise**

```
noiseLevel = 0.01 * Input["Percentage of noise?"]
```

```
0.005
```

```
If[
  noiseLevel == 0,
  (*the number of exc itations (spins up) is invariant*)
  (*we may reduce the size of the basis*)
  chosenFew = Select[statesBasis, Count[#, 1] == numberSpinsUp &];
sizeBasis = Length[chosenFew];
  ,
  chosenFew = statesBasis; (*cool name, a bit out of date, but...*)
sizeBasis = numberStates;
 ];
```

```
sizeBasis
```

```
8
```

Hamiltonian

▪ Definition of the Hamiltonian

Note that here no interaction term is included since the double occupancy term is diagonal in each subspace. The respective energy has to be added to the eigenvalues.

```
H = Function[
   state,
   Expand[
    Jxy
      Sum[
       z[
         FlipUp[k, FlipDown[k + 1, state]]
        ]
        + z[
         FlipDown[k, FlipUp[k + 1, state]]
        ],
       {k, 1, sites - 1}
      ]
     + Jz
      Sum[
       Sum[
        z[
          n[k, sigma, n[k + 1, sigma, state]]
         ]
         - z[
          n[k, sigma, n[k + 1, Bar[sigma], state]]
         ],
        {sigma, 0, 1}],
       {k, 1, sites - 1}
      ]
   ]
  ];
```

▪ defining the hamiltonian matrix in the subspace with a given occupancy number

The following instruction defines the subspaces of states used in the diagonalization.

Now, one has to apply the hamiltonian to all states in the basis. The hamiltonian matrix is defined doing the scalar product between the previous result and again the the vectors of the basis. Each matrix entry is defined by ⟨basis vector|H| basis vector⟩.

```
hlist = Table[H[chosenFew[[j]]], {j, sizeBasis}];
```

```
h = (
   Table[
    scalarproduct[
     z[chosenFew[[i]]],
     hlist[[j]]
    ],
    {i, sizeBasis},
    {j, sizeBasis}
   ]
  );(*MatrixForm[h]*)
```

▪ adding noise

Values of Jz and Jxy

```
JzReal = 100.;
JxyReal = 2.;

hXXZ = h /. {Jz → JzReal, Jxy → JxyReal};
hNoise = ConstantArray[0, Dimensions[hXXZ]];

If[
 noiseLevel ≠ 0,
 maxNoise = Min[Abs[JzReal], Abs[JxyReal]] * (1 + I) * noiseLevel;
hNoise = PadRight[
   Table[
    RandomComplex[{-maxNoise, maxNoise}],
    {n, sizeBasis},
    {i, n}],
   {sizeBasis, sizeBasis}
  ];
hNoise = hNoise + ConjugateTranspose[hNoise];
]

hReal = hXXZ + hNoise;

HermitianMatrixQ[hReal]
```

```
True
```

▪ diagonalizing and checking for degenerate energy gaps

```
egvalues = HandyEgvalues[hReal];

egstates = HandyEgvectors[hReal];

degenerateEnergyGaps = DegenerateGaps[egvalues]
```

```
False
```

Basis

▪ Rotation matrices and functions

```
can2energyMatrix = Transpose[egstates] ;

energy2canMatrix  =  Chop[Inverse[can2energyMatrix]];
```

```
Can2En = Function[
   matrixCan,
   Chop[
    energy2canMatrix . matrixCan . can2energyMatrix
    ]
  ];
```

```
En2Can = Function[
   matrixEn,
   Chop[
    can2energyMatrix . matrixEn . energy2canMatrix
    ]
  ];
```

Evolution of the density matrix

- ### Inital, pure state, density matrix

```
PureDensity = Function[
   pim,
    Table[
     If[i == j && i == pim, 1, 0 ],
     {i, sizeBasis},
     {j, sizeBasis}
    ]
  ];
```

- ### Evolution of the density matrix

```
EvolutionMatrix = Function[
   t,
   Table[
    If[
     i == j ,
     Exp[-I * egvalues[[i]] * t ],
     0
    ],
    {i, sizeBasis}, {j, sizeBasis}
   ]
  ];
```

```
EvolutionEn = Function[
   {startingDensityEn , t},
       Chop[
            EvolutionMatrix[t] .
             startingDensityEn .
             ConjugateTranspose[
              EvolutionMatrix[t]
               ]
             ]
  ];
```

Time Evolution of Entropy Measures - a Crude Simulation

We start with a simple system : the first spins of the chain are down and the last ones are up

- ### Inicializing

- **Parameters**

```
sitesSubsystem = Input["Number of sites of the subsystem?"]
```

```
1
```

```
positionSubsystem =
 Input["Position of the subsystem in the chain? 0: beggining, 1: middle"]
```

```
1
```

```
(*epsilon = Input["Epsilon (for the smooth entropies)?"]*)
epsilon = 0.005
```

```
0.005
```

```
timeStep = Input["Time step?"]
```

```
0.0001
```

```
finalTime = Input["Total time of simulation?"]
```

```
20
```

```
numberSteps = Ceiling[finalTime / timeStep]
```

```
200 000
```

- **Vectors**

```
vonNeumannEntropy1 = Table[0, {i, numberSteps}];

minEntropy1 = Table[0, {i, numberSteps}];
maxEntropy1 = Table[0, {i, numberSteps}];

renyi05Entropy1 = Table[0, {i, numberSteps}];
renyi2Entropy1  = Table[0, {i, numberSteps}];

smoothMinEntropy1  =  Table[0, {i, numberSteps}];
smoothMaxEntropy1  =  Table[0, {i, numberSteps}];

distance2InitialState =  Table[0, {i, numberSteps}];
distance2AverageState =  Table[0, {i, numberSteps}];
```

- **Debug**

```
debugTime = False;
```

```
time2debug = Min[Floor[numberSteps / 100], 10 000]
```

```
2000
```

```
ii = 1;

jj = 1;
```

Initial density matrix, reduced density matrix and eigenvalues

```
(*it is starting in state 11111000000000 (the number of ones is numberSpinsUp) *)

pim = 1;

pim = Switch[Input[
   "How should we choose our initial state?
a - all the spins up, then all the spins down;
b - random initial product state;
c - spins of the subsystem up, all the others down"],
  a,
  Position[chosenFew, ExcitedSubsystem[sites, numberSpinsUp, 0]][[1]][[1]],
  b,
  RandomInteger[{1, sizeBasis}],
  c,
  Position[chosenFew,
     ExcitedSubsystem[sites, sitesSubsystem, positionSubsystem]][[1]][[1]]
 ]

2

initialDensityCan = PureDensity[pim];

initialDensityEn = Can2En[initialDensityCan];

temp1 =
  ReducedSystem[initialDensityCan, chosenFew, sites, sitesSubsystem, positionSubsystem] ;

initialReducedDensity = temp1[[1]];

reducedBasis = temp1[[2]];

copyInitialDensityEn = initialDensityEn;

copyInitialReducedDensity = initialReducedDensity;
```

Auxiliar matrices

```
finalDensityEn = ConstantArray[0, Dimensions[initialDensityEn]];

finalDensityCan = ConstantArray[0, Dimensions[initialDensityEn]];
```

Average density matrices

```
bigTimeStep = 10;

longFinalTime = 1 000 000;

shortNumberSteps = Ceiling[longFinalTime / bigTimeStep]

100 000

averageReducedDensity = copyInitialReducedDensity;
averageDensityCan = initialDensityCan;
averageDensityEn = initialDensityEn;
```

```
DateString[]

Sun 5 Jul 2009 03:20:50

ProgressIndicator[Dynamic[jj], {1, shortNumberSteps}]

Do[
  finalDensityEn =
   EvolutionEn[
    initialDensityEn,
    bigTimeStep + RandomReal[{-bigTimeStep / 10., bigTimeStep / 10.}]
   ];

  finalDensityCan = En2Can[finalDensityEn];

  temp1 = ReducedSystem[finalDensityCan,
    chosenFew, sites, sitesSubsystem, positionSubsystem] ;

  averageReducedDensity = averageReducedDensity + temp1[[1]];
  averageDensityCan = averageDensityCan + finalDensityCan;
  averageDensityEn = averageDensityEn + finalDensityEn;

  initialDensityEn = finalDensityEn;

  ,
  {jj, shortNumberSteps}
 ];

averageDensityEn = Chop[averageDensityEn / (shortNumberSteps + 1)];

averageDensityCan =  Chop[averageDensityCan / (shortNumberSteps + 1)];

averageReducedDensity  = Chop[averageReducedDensity / (shortNumberSteps + 1)];
```

Properties of the average reduced density matrix

```
MatrixForm[averageReducedDensity]
```

$$\begin{pmatrix} 0.0838058 & -0.0000124349 - 0.0000395689\,i \\ -0.0000124349 + 0.0000395689\,i & 0.916167 \end{pmatrix}$$

```
DateString[]

Sun 5 Jul 2009 03:24:57

averageEgvalues = HandyEgvalues[averageReducedDensity];

DateString[]

Sun 5 Jul 2009 03:24:57

avgVonNeumannEntropy = VonNeumannEntropyEg[averageEgvalues];

avgMinEntropy = MinEntropyEg[averageEgvalues];

avgMaxEntropy = MaxEntropyEg[averageEgvalues];

avgRenyi05Entropy = RenyiEntropyEg[0.5, averageEgvalues];

avgRenyi2Entropy = RenyiEntropyEg[2, averageEgvalues];
```

```
avgSmoothMinEntropy = SmoothMinEntropyEg[averageEgvalues, epsilon];
```

```
avgSmoothMaxEntropy = SmoothMaxEntropyEg[averageEgvalues, epsilon];
```

```
distanceInitialAverageReduced =
  TraceDistance[averageReducedDensity, copyInitialReducedDensity];
```

- **Exporting data**

```
ExportList["ReducedBasis", reducedBasis];
```

```
ExportList["GlobalBasis", chosenFew];
```

```
Export["AverageDensityCan.dat", averageReducedDensity + 0.0 ];
```

```
Export["Re_AverageReducedDensity.dat", Re[averageReducedDensity + 0.0 ]];
```

```
Export["Im_AverageReducedDensity.dat", Im[averageReducedDensity + 0.0 ]];
```

```
Export["Re_InitialReducedDensity.dat", Re[ initialReducedDensity + 0.0]];
```

```
Export["Im_InitialReducedDensity.dat", Im[ initialReducedDensity + 0.0]];
```

```
propAvgDensityMatrix = {
   "properties of the average reduced density matrix",
   " ",
   "size", sizeBasis,
   "Von Neumann Entropy ", avgVonNeumannEntropy + 0.0,
   "Min Entropy ", avgMinEntropy + 0.0,
   "Max Entropy ", avgMaxEntropy + 0.0,
   "Renyi 2 Entropy ", avgRenyi2Entropy + 0.0,
   "Renyi 0.5 Entropy" , avgRenyi05Entropy + 0.0,
   "Smooth Min Entropy ", avgSmoothMinEntropy + 0.0,
   "Smooth Max Entropy ", avgSmoothMaxEntropy + 0.0,
   "Distance between initial and average reduced states ",
   distanceInitialAverageReduced + 0.0
  };
```

```
Export["PropertiesAverageDensityMatrix.txt", propAvgDensityMatrix]
```

```
PropertiesAverageDensityMatrix.txt
```

```
FilePrint["PropertiesAverageDensityMatrix.txt"]
```

The great Do cicle

```
initialDensityEn = copyInitialDensityEn;
```

Here the time step is always the same, and so is the evolution matrix

```
evolutionMatrix = EvolutionMatrix[timeStep];
```

```
initialReducedDensity = copyInitialReducedDensity;
```

```
averageReducedDensity =
  Import["Re_AverageReducedDensity.dat"] + I Import["Im_AverageReducedDensity.dat"];
```

```
ProgressIndicator[Dynamic[ii], {1, numberSteps}]
```

```
Do[
  (*finalDensityEn=EvolutionEn[initialDensityEn,timeStep];*)
  finalDensityEn = Chop[
    evolutionMatrix .
     initialDensityEn .
     ConjugateTranspose[
      evolutionMatrix
     ]
   ];

  finalDensityCan = En2Can[finalDensityEn];

  temp1 = ReducedSystem[finalDensityCan,
    chosenFew, sites, sitesSubsystem, positionSubsystem] ;
  subDensity1 = temp1[[1]];
  (*subDiagonal1=MakeDiagonal[HandyEgvalues[subDensity1]];*)
  subEgvalues1 = HandyEgvalues[subDensity1];

  vonNeumannEntropy1[[ii]] = VonNeumannEntropyEg[subEgvalues1];

  minEntropy1[[ii]] = MinEntropyEg[subEgvalues1];
  maxEntropy1[[ii]] = MaxEntropyEg[subEgvalues1];

  renyi05Entropy1[[ii]] = RenyiEntropyEg[0.5, subEgvalues1];
  renyi2Entropy1[[ii]] = RenyiEntropyEg[2, subEgvalues1];

  smoothMinEntropy1[[ii]] = SmoothMinEntropyEg[subEgvalues1, epsilon];
  smoothMaxEntropy1[[ii]] = SmoothMaxEntropyEg[subEgvalues1, epsilon];

  distance2InitialState[[ii]] = TraceDistance[initialReducedDensity, subDensity1];
  distance2AverageState[[ii]] =  TraceDistance[averageReducedDensity, subDensity1];

  initialDensityEn = finalDensityEn;
  ,
  {ii, 1, numberSteps}
 ];
```

```
DateString[]
```

```
Sun 5 Jul 2009 03:36:30
```

- **Exporting data**

```
ExportList["Distance2Initial", distance2InitialState];
```

```
ExportList["Distance2Average", distance2AverageState];
```

```
ExportList["SmoothMin", smoothMinEntropy1];
```

```
ExportList["SmoothMax", smoothMaxEntropy1];
```

```
ExportList["Min", minEntropy1];
```

```
ExportList["Max", maxEntropy1];
```

```
ExportList["Renyi05", renyi05Entropy1];
```

```
ExportList["Renyi2", renyi2Entropy1];
```

```
ExportList["VonNeumann", vonNeumannEntropy1];
```

Parameters

```
parameters = {
   "xz model", " ",
   "* chain properties *",
   "total number of sites", sites,
   "number of spins up", numberSpinsUp,
   "size of the basis", sizeBasis,
   "number of sites of the subsystem", sitesSubsystem,
   "position of the subsystem on the chain", positionSubsystem,
   " ", "* hamiltonian properties *",
   "Jxy", JxyReal,
   "Jz", JzReal,
   "Percentage of noise", 100 * noiseLevel,
   "Degenerate energy gaps", degenerateEnergyGaps,
   " ", "* simulation properties *",
   "epsilon", epsilon,
   "time step", timeStep,
   "total time of simulation", finalTime,
   "number of steps", numberSteps,
   " ", "* for the average density matrix *",
   "time step", bigTimeStep,
   "total time of simulation", longFinalTime,
   "number of steps", shortNumberSteps,
   " ",
   "started at", startingTime,
   "finished at", DateString[]
  };
```

```
Export["parameters.txt", parameters]
```

```
parameters.txt
```

```
FilePrint["parameters.txt"]
```

```
DateString[]
```

```
Sun 5 Jul 2009 03:37:16
```

```
Directory[]
```

```
/home/lidia/Documents
```