Thermalization and equilibration in quantum many-body systems: Insights from free models

Bachelor Thesis

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1 Introduction

Leaving the house on a cold winter day will soon cause a feeling of cold, despite your body's effort to stay warm. This is due to a phenomenon called "thermal equilibration" that will inevitably drive your body temperature towards the temperature of the environment. The study of systems in thermal equilibrium, equilibrium thermodynamics, has a long and successful tradition in physics. It is also known for a long time that most systems in thermal equilibrium are well described by the Gibbs distribution, or canonical ensemble, of statistical mechanics. The Gibbs distribution is a probability distribution for the probabilities p_j to find a system in a state with energy E_j. The probabilities p_j are given by

$$p_j = \frac{1}{Z} e^{-\beta E_j},$$

where the constant $Z = \sum_j e^{-\beta E_j}$ is called the *partition function* and ensures that the probabilities add up to unity and $\beta = \frac{1}{k_B T}$ is the inverse temperature. Here k_B is the Boltzmann-constant. In quantum mechanics the Gibbs distribution is represented by a

mixed state with probabilities p_j to find the system in an eigenstate with energy E_j. This state is usually called the Gibbs state.

The Gibbs distribution maximizes the entropy $S = -\sum_j p_j \log p_j$ under the constraint that the expectation value of the energy is fixed to a certain value. In fact, in statistical mechanics, roughly speaking, this state serves as a *definition* of temperature. If a system is in an equilibrium state that is well described by the Gibbs distribution we say it has *thermalized*.

In classical physics the validity of using the Gibbs distribution to describe systems in thermal equilibrium follows from the micro canonical postulate. This postulate says that all microscopic states that are compatible with the macroscopic state are equally likely to be realized (see any standard text-book on statistical mechanics, for example ref. [1, 2]).

This probabilistic description cannot result naturally in classical physics because classical physics is completely deterministic. Any probabilistic description of a system therefore has to enter because of subjective lack of knowledge about the system. Thus the validity of the use of the Gibbs distribution has to follow from some external postulate.

If quantum theory is a fundamental and true description of the universe that does not need any external postulates, the conditions for the validity of the use of the Gibbs distribution must be derivable from quantum mechanics. One approach to this derivation is called "Pure state quantum statistical mechanics" (for a recent review see [3]). The basic idea is that the universe is ideally in a pure state Ψ and by looking only at a small part of the universe one sees a mixed state of that part, which is very close to the Gibbs state. The entropy plays a very different role in this case [4]: In classical statistical mechanics the entropy is not a property of the state of the system but a measure of our lack of knowledge about the state of the system. In contrast to this, in the case of quantum mechanics the Gibbs state results as the reduction of a pure state of a larger quantum system. The entropy is not a measure of lack of knowledge about the state of the system that is caused by our inability to completely measure the state of the system, but results from entanglement. Even if we had perfect knowledge about the pure state of the universe, the entropy of a subsystem would be non-zero if the universe is not in a product state of the subsystem and the rest of the universe.

In recent time there has been a lot of progress on rigorously showing when a subsystem of a large generic system equilibrates [4, 5, 6, 7, 8] and if it does or does not thermalize [9, 10].

It is interesting however not only to know if systems thermalize but also which process is ultimately responsible for this behavior. In this thesis I investigate whether a certain conjectured process of thermalization, the *Eigenstate Thermalization Hypothesis* (see section 2.2.1), holds for two spin models which can be mapped to free fermionic models.

Furthermore I will study the role that conserved quantities play in the process of equilibration.

1.1 Structure of the document

In section 2 I give a very brief review of recent results about the equilibration and thermalization of subsystems of large generic systems and discuss the role of conserved quantities in the process of equilibration from a general point of view. Section 3 introduces spin and fermionic models. In section 4 I introduce the first model and discuss the role of conserved quantities in equilibration for this model. I also discuss whether the Eigenstate Thermalization Hypothesis (ETH) holds. Using numerical results the ETH is studied from the viewpoint of the XX-model in section 5. Throughout the whole document I will set $\hbar = 1$.

2 Equilibration and thermalization

In this section I will give a brief review of equilibration and thermalization and some recent important results in understanding these mechanisms from a quantum mechanical point of view. Importantly, these results do not make use of artificial concepts like ensemble averages which can be found in almost all text-books on statistical mechanics.

As mentioned in the introduction, roughly speaking, thermalization means equilibration towards the Gibbs state. While we know from experience that most systems in nature will evolve towards such a state it is quite difficult to precisely formulate when and how this happens. As discussed in [6] it is useful to split the problem into different parts, dealing with equilibration separately from thermalization. We begin with equilibration.

We first define the time-average and trace-distance as they will be used often throughout this section.

Definition 1 (Time-Average) The time average ω of a state described by a density matrix $\rho(t)$ is defined as

$$\omega = \langle \rho(t) \rangle_t = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \rho(t) \, \mathrm{d}t. \tag{1}$$

□

Definition 2 (Trace-distance) The trace-distance of two states ρ_1 and ρ_2 is defined as

$$\mathcal{D}(\rho_1, \rho_2) = \frac{1}{2}\mathsf{Tr}\left(\sqrt{(\rho_1 - \rho_2)^2} \right) \tag{2}$$

$$= \max_{0 \le A \le \mathbb{1}} \left(\mathsf{Tr}\left(A\rho_1 \right) - \mathsf{Tr}\left(A\rho_2 \right) \right), \tag{3}$$

where the maximization is taken over Hermitian operators. Note that the trace-distance directly measures the physical distinguishability.

□

2.1 Equilibration

As equilibration is a necessary condition for thermalization I first review what equilibration means in a quantum mechanical system and how it can be described mathematically. Let me stress that equilibration is not sufficient for thermalization: A system that thermalizes has to equilibrate but a system that equilibrates must not necessarily equilibrate towards its Gibbs state.

In classical physics, or generally in what is usually called a dynamical system, an equilibrium state is a state that does not change over time. Due to the unitary evolution of a closed quantum mechanical system, however, a pure state of a closed system will never equilibrate in the sense that it does not change over time at all. The only exception to this is the situation when the system starts in an eigenstate of its Hamiltonian. Therefore it is necessary to introduce a more general notion of equilibration in quantum systems. A first guide into a more general notion of equilibration is that generally only certain observables A can be measured, but not the state itself. In accordance to recent literature (see for ex. [6, 9, 10]) I will therefore say that an observable equilibrates if its expectation value $\langle A \rangle = \mathsf{Tr}\left(A\rho(t) \right)$ is close to its time-average for most times t. Often it is only possible to measure local observables with a support only on a small part of the system. It therefore makes sense to say that a subsystem equilibrates if all observables with support only on this subsystem equilibrate. Mathematically, this condition is equivalent to saying that the trace-distance of the state of the subsystem ρ_S to its time-average $\omega_S = \mathsf{Tr}_B\left(\omega \right)$ is very small for most times. Note that an equilibrium state of a system is in general not independent of the initial state of the system and therefore generally not unique. For example all the eigenstates of the Hamiltonian have different equilibrium states, namely themselves.

This notion of equilibration does not require that the equilibrium state commutes with the Hamiltonian of the system, although, of course, every state that commutes with the Hamiltonian is an equilibrium state. In this sense, the definition therefore agrees with the classical definition. Furthermore I want to stress that if a state equilibrates then, by definition, it has to equilibrate to its time-average.

Using this notion of equilibration one can now ask if and when subsystems of bigger system equilibrate. The following results by Linden et al. [6] show that most subsystems of large enough systems in fact do equilibrate. The guiding idea is to think of a small system with limited degrees of freedom that is in contact with a large heat bath which has very many degrees of freedom. Thus consider a large system partitioned into a (small) *subsystem*, with Hilbert-space $\mathcal{H}_S$ of dimension d_S, and a (large) *bath*, with Hilber-space $\mathcal{H}_B$ of dimension d_B. The partition of the total system can be completely arbitrary as long as the subsystem is much smaller then the bath. The complete Hilbert space is then given by the tensor product $\mathcal{H}_S \otimes \mathcal{H}_B$. Let the Hamiltonian of the total system be given by $H = \sum_k E_k |E_k\rangle\langle E_k|$, where $|E_k\rangle$ are the eigenstates of the Hamiltonian. Linden et al. also assume that the Hamiltonian has *non-degenerate energy-gaps*. This assumption already appeared in a paper by von Neumann [11] and states that for any four eigenstates E_k, E_l, E_m, E_n we have that $E_k - E_l = E_m - E_n$ implies $k = l$ and $m = n$ or $k = m$ and $l = n$. This a very weak condition, because any small random perturbation ensures this condition, and can be viewed as an ergodicity condition. For generic large systems in nature we can therefore assume that it holds.

A pure state of the total system is given by

$$|\Psi(t)\rangle = \sum_k c_k e^{-iE_k t} |E_k\rangle$$

with density matrix $\rho = |\Psi(t)\rangle\langle\Psi(t)|$. The state of the subsystem ρ_S is given by tracing out the bath, so $\rho_S = \mathsf{Tr}_B(\rho)$ and correspondingly $\rho_B = \mathsf{Tr}_S(\rho)$. The dynamics of the subsystem are governed by the dynamics of the total system as

$$\rho_S(t) = \mathsf{Tr}_B(\rho(t)).$$

Particularly the subsystem does not evolve under unitary evolution governed by its Hamiltonian H_S.

Due to the non-degenerate energy-gaps the time-averaged density matrix of the total system is simply given by

$$\omega = \sum_k |c_k|^2 |E_k\rangle\langle E_k|.$$

The time-average of the subsystem is $\omega_S = \mathsf{Tr}_B(\omega)$. A convenient quantity is the *effective dimension* of a state defined as follows.

Definition 3 (Effective dimension [6]) The effective dimension of a state $|\Psi(t)\rangle$, as defined above, with a time-average density matrix ω is given by

$$d^{\mathsf{eff}}(\omega) = \frac{1}{\mathsf{Tr}(\omega^2)} = \frac{1}{\sum_k |c_k|^4}. \tag{4}$$

□

The statement that subsystems usually equilibrate can then be made precise by the following theorem.

Theorem 1 (Equilibration of subsystems [6]) *Let* $\Psi \in \mathcal{H}$ *evolve under a Hamiltonian with non-degenerate energy gaps. Then the average distance of the state of any subsystem* ρ_S *to its time-average* ω_S *is bounded as*

$$\langle \mathcal{D}(\rho_S(t), \omega_S)\rangle_t \leq \frac{1}{2}\sqrt{\frac{d_S}{d^{\mathsf{eff}}(\omega_B)}} \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\mathsf{eff}}(\omega)}}.$$

□

The theorem says that a subsystem equilibrates as long as the effective dimension explored by the bath is much bigger then the dimension of the subsystem's Hilbert-space.

In ref. [6] it is also shown that for most pure states of the total system the effective dimension is very large, even in the case of a very small uncertainty in the energy. Furthermore the authors show that almost all states chosen from a large restricted subspace of $\mathcal{H}$ give (almost) the same time-averaged state. This shows that the equilibrium value is fairly independent of the initial state.

2.1.1 The role of conserved quantities

From classical physics we know that conserved quantities, or integrals of motion, are very important in the evolution of dynamical systems. Conserved quantities are, in the classical case, quantities that do not change over time. The reason for the importance of these quantities in the evolution of a system is intuitively very clear: Once the values of all conserved quantities are fixed they cannot change anymore. If there are a lot of conserved quantities the system can therefore only access a very small subset of all possible states. This means that the state of a system depends a lot on the initial conditions if there are many conserved quantities. In quantum mechanical systems the situation is different as observables are not given by real numbers but by Hermitian operators. Measuring these operators can lead to different outcomes even when the system is in the same state.

I will now discuss how conserved quantities can be defined in quantum systems and how they influence the equilibration of a system.

Let us define that a conserved quantity is an observable whose expectation value does not change under the unitary evolution of the system. The condition for this is that the observable commutes with the Hamiltonian. In general it is useful to distinguish *local* and *global* conserved quantities. To discuss these, consider a system partitioned into a subsystem, described by a Hilbert-space $\mathcal{H}_S$ and a bath, described by a Hilbert-space $\mathcal{H}_B$. The total Hilbert-space is again $\mathcal{H}_S \otimes \mathcal{H}_B$. The Hamiltonian governing the dynamics of the system may be written as $H = H_S + H_B + H_{SB}$ where H_S and H_B only act on the system and bath, respectively, and H_{SB} contains the interactions. A *local* conserved quantity is an observable that commutes with the Hamiltonian of the *total* System but only has support on a subsystem, i.e. it is of the form $A = A_S \otimes \mathbb{1}$. A *global* conserved quantity is a conserved quantity that acts non-trivially on the total system.

There is ongoing debate about the role of local and global conserved quantities in the process of equilibration and thermalization, therefor I would like to list some facts about the role of conserved quantities in equilibration. Some of these might seem trivial but nonetheless it is important to state them. The first important point to make is that the expectation values of conserved quantities do not change over time. Therefore they are fixed by the initial conditions and the evolution of the total closed system is restricted to a subset of states. This has important consequences for equilibration. It was shown in ref. [9] that the equilibrium state of any initial state has to be the one that maximizes its entropy while keeping the expectation values of all conserved quantities fixed. As this is a very important insight let me reproduce the proof here.

PROOF (EQUILIBRATION TO MAXIMUM ENTROPY STATE [9]) Let $P_j = \sum_{k \in I_j} |E_k\rangle\langle E_k|$ be the projectors onto the (possibly degenerate) subspaces of the Hamiltonian $H = \sum_k E_k |E_k\rangle\langle E_k|$. The sets I_j collect the different eigenstates with same energy, so $E_k = E_l$ if $k, l \in I_j$. Then the time average of a state $\rho(t) = \sum_{j,k} c_j c_k^* e^{-i(E_j - E_k)t} |E_j\rangle\langle E_k|$ is clearly given by

$$\omega = \sum_j P_j \rho(t) P_j. \tag{5}$$

As the von Neumann entropy is Schur-concave it follows directly by the Pinching Lemma

(see ref. [12]) that this is the state with maximum entropy that gives the same expectation values as $\rho(t)$ of all conserved quantities. ∎

Given all conserved quantities this state can be calculated fairly easy. To do this let G be a linear basis of the conserved quantities. Thus, every conserved quantity can be written as a linear combination of the elements of G. Let the total system be described by a finite-dimensional Hilbert-space $\mathcal{H}$. Then $|G|$, the number of elements in G, is finite. Now suppose the system is initially in some state ρ, which can be mixed or pure. Then all the expectation values $\langle G_\alpha \rangle_\rho = \text{Tr}(\rho G_\alpha)$ of the conserved quantities $G_\alpha \in G$ with respect to ρ are fixed. The evolution of the system is then restricted to the set of states

$$\{\sigma \mid \text{Tr}(\sigma G_\alpha) = \langle G_\alpha \rangle_\rho \quad \alpha = 1, \ldots, |G|\}.$$

Then the state with maximum von Neumann entropy in this set is given by

$$\omega = \frac{1}{Z} e^{-\sum_\alpha \lambda_\alpha G_\alpha}, \tag{6}$$

where the factor Z ensures $\text{Tr}(\omega) = 1$ and the constants λ_α are chosen in such a way that the expectation values of the conserved quantities fulfill $\langle G_\alpha \rangle_\omega = \langle G_\alpha \rangle_\rho$.

PROOF (STATE WITH MAXIMUM ENTROPY) The proof is almost exactly the same as the proof of extremality of the entropy of the canonical ensemble as found in [1]. The only difference is the number of expectation values that are fixed. Let the relative entropy given by

$$S(\sigma \| \rho) = \text{Tr}(\sigma(\ln \sigma - \ln \rho)) \geq 0, \tag{7}$$

see for example [13]. Let σ be a state with the same expectation values for the conserved quantities G_α as ω and otherwise arbitrary. The von Neumann entropy of ω is

$$S(\omega) = \ln Z + \sum_\alpha \lambda_\alpha \langle G_\alpha \rangle_\omega.$$

From eq. 7 it follows that

$$\begin{aligned} S(\sigma) &\leq \text{Tr}(\sigma \ln \rho) \\ &= \ln Z + \sum_\alpha \lambda_\alpha \langle G_\alpha \rangle_\sigma = S(\omega), \end{aligned}$$

because we required $\langle G_\alpha \rangle_\sigma = \langle G_\alpha \rangle_\omega$. ∎

The state ω was conjectured to be the equilibrium state of a system, if it equilibrates at all, and called the *Generalized Gibbs Ensemble (GGE)* by Rigol et al. [14, 15, 16]. By the preceding argument it is clear that it has to be this one.

The number of conserved quantities of a system grows exponentially with the system size. This is due to the fact that the Hilbert-space grows exponentially with the system size. Given all conserved quantities of a system together with their initial expectation values it is therefore easy to write down the equilibrium state ω symbolically. From a computational point of view however it is very difficult to calculate this state. An interesting question to ask is therefore whether it is really necessary to consider *all* conserved quantities of the total system if one is only interested in the behavior of some small subsystem. It is imaginable that the equilibrium value of a subsystem does not depend on the expectation values of observables that only act on different subsystem very far away. One of the main results of this thesis is that this is indeed the case for a certain spin-model.

The question of the role of conserved quantities in equilibration is also closely connected to the notion of integrability, both in classical as well as in quantum mechanics. While

integrability is a well defined concept in classical systems it is quite difficult to define in the quantum mechanical setting. In fact there are multiple different definitions in the quantum case. They range from the notion that a system is integrable if it can be solved to the requirement of certain sets of conserved quantities. For a recent discussion see [17]. Until recently there seemed to be a consensus that non-integrable systems thermalize and systems that are integrable do not thermalize. Especially if there is no well-defined concept of integrability such a statement has to be questioned and it was indeed shown that there are non-integrable system that do not thermalize [9]. Furthermore, in ref. [18] it was shown that there is a large class of integrable systems that locally relax to an equilibrium state. In this class of systems it is even possible to compute the exact time-window in which it happens.

Concluding we can say that the results by Linden et al showed that equilibration is a common feature of subsystems of large quantum systems. Conserved quantities play an important role in the process of equilibration play because they restrict the dynamics to a smaller subset of states. Given all conserved quantities and their expectation values it is possible to calculate directly the equilibrium state. In this thesis I study if the equilibrium state of a subsystem can also be computed with incomplete knowledge of the conserved quantities, i.e. when only the expectation values of the local conserved quantities on the subsystem are known. We will see a model where it is sufficient to know the expectation values of the local conserved quantities that only have support on the subsystem together with its boundary.

2.2 Thermalization

We speak of thermalization of a (sub)-system if it equilibrates and can be well described by the Gibbs state

$$\rho_{\text{Gibbs}} = \frac{1}{Z} e^{-\beta H_{\text{S}}},$$

where H_{S} is the Hamiltonian describing the dynamics of the system. This formula is used to calculate expectation values of observables for systems at finite temperature. The results of calculations with this formular are often in very good agreement with experiments. It is therefore of fundamental interest and importance to understand when and why the Gibbs state gives a good description of a system's state. In this section I briefly discuss recent results that show that a large class of quantum mechanical systems can be expected to thermalize.

The results by Linden et al [6], summarized in section 2.1, show that equilibration is a very common property for generic systems. Equilibration alone, however, does not have to lead to a state that is locally well described by the Gibbs state. Although the Gibbs state looks very similar to the state defined in eq. 6 it is in general not such a state. In fact the subsystem's Hamiltonian is in general not even a conserved quantity. Therefore the equilibration results do not show that thermalization generally occurs.

Recently, however, Riera et al. proved [10] that quantum mechanical systems thermalize under very general conditions. Like Linden et al. they consider a large closed system partitioned into a subsystem and a bath. Their first assumption is that the Hamiltonian of the total system has non-degenerate energy gaps. Furthermore they require that the interaction between the subsystem and the bath is sufficiently weak. Unlike in the case of traditional perturbation theory, sufficiently weak here means that the infinite-norm of the interaction-Hamiltonian has to be much smaller than the uncertainty Δ in the energy E of the state of the total system. Traditional perturbation theory is usually only useful if the perturbation is small compared to the *gaps* between the eigenvalues of the Hamiltonian. In macroscopic systems these gaps can become exponentially small, therefore this new condition of sufficiently weak interactions is much more realistic.

The last assumption is that the density of states of the bath can be approximated well by an exponential. For generic, non-degenerate, large systems this is a very common feature which essentially already follows from combinatorics.

Riera et al. then show that starting with a state with uniform overlap to eigenstates of the total Hamiltonian that have energy inside the interval $[E, E + \Delta]$ and zero overlap outside that interval, a subsystem's state equilibrates toward its Gibbs state. In particular this result shows that a micro canonical state is locally well described by a Gibbs state.

For generic large systems we can therefore expect that small subsystems can be well described by the Gibbs state.

Note that when thermalization occurs, the subsystem has to equilibrate to a state that is fairly independent of the initial state of both the subsystem and the bath.

2.2.1 Eigenstate Thermalization Hypothesis

Ultimately the arguments for thermalization are a combination of measure-theoretic arguments and perturbation arguments. Thereby they do not show what process is responsible for the approach to thermal equilibrium. There are a number of proposed processes that can explain thermalization, but, so far, none of them could be proven to hold in general. One of them, the so-called *Eigenstate Thermalization Hypothesis (ETH)*, has received a lot of attention recently [14, 15, 19, 20]. It was first proposed independently by Deutsch and Srednicki [21, 22]. Here, I give the definition of ref. [15], which I will call the *strong ETH*: Let A be any local observable with support only on a small subsystem, of maximal size m, and $|E_n\rangle$ an eigenstate with energy E_n. Then the ETH holds if the expectation value of A with respect to $|E_n\rangle$ equals the expectation value of A with respect to a micro canonical ensemble with mean energy E_n:

$$\langle E_n | A | E_n \rangle = \langle A \rangle_{\text{m.c.}} \quad \forall A \text{ with support } \leq m.$$

There is some ambiguity in this definition as it does not specify the energy-uncertainty of the micro canonical ensemble. Obviously the ETH holds if the energy-uncertainty is zero because then the micro canonical ensemble is just the eigenstate $|E_n\rangle$. In experimental conditions, of course, the energy-uncertainty is given by the ability of an experimentalist to prepare the state of the system. For macroscopic systems it will therefore include a big number of eigenvalues of the Hamiltonian of the total system.

If we combine the ETH with the results of Riera et al., summarized in the last section, we can expect that any system that fulfills the ETH can locally be well described by the Gibbs state if it is in an eigenstate. With the additional assumption that the temperature of the local Gibbs state is almost the same for two eigenstates which have almost the same energy, any state with small energy uncertainty could locally be well described by the Gibbs state. The assumption about the relation between the local temperature and the global energy is necessary, because a sum of two Gibbs states with different temperatures is in general not a Gibbs state, so the Gibbs states of a system do not form a convex set. If the assumption, that the inverse temperature depends smoothly on the total energy, holds, the ETH could be considered as a plausible explanation of thermalization, already on the level of eigenstates.

This is a very strong formulation of the ETH. In the original work by Srednicki the author does not claim that *all* local observables behave in the way described above, but only conjectures this to be true for the momentum of the particles of a hard-sphere gas. However, one could hope that the hypothesis generalizes to a more general setting.

An additional point I want to make is that the question if the strong ETH can hold, is connected to the topic of local and global conserved quantities. To see this, suppose we are given two eigenstates $|E_1\rangle, |E_2\rangle$, with energies $E_1 \approx E_2$, of the Hamiltonian H of the total system. The strong ETH then implies that for all *local* observables A, with a support

that is small enough, we have

$$\langle E_1 \,|\, A \,|\, E_1 \rangle = \mathsf{Tr}\left(A\rho^{\mathsf{S}}_{\mathsf{Gibbs}}(\beta_1) \right) \cong \mathsf{Tr}\left(A\rho^{\mathsf{S}}_{\mathsf{Gibbs}}(\beta_2) \right) = \langle E_2 \,|\, A \,|\, E_2 \rangle,$$

where $\rho^{\mathsf{S}}_{\mathsf{Gibbs}}(\beta_j)$ is the Gibbs state of the subsystem, with inverse temperature β_j, when the total system has energy E_j. It therefore implies, that if we fix the expectation value of the global conserved quantity H, the expectation values of all local observables on a small enough subsystem are fixed. This also includes conserved quantities. In such a system the expectation values of the local conserved quantities therefore cannot be independent of the expectation value of the Hamiltonian of the system. Concluding, a sufficient condition to falsify the strong ETH, for subsystems up to size m, is the existence of a set of local measurements, with support of size at most m, that can distinguish two eigenstates of H which have almost the same energy.

In this thesis we will see one model where it is possible to show analytically that the strong ETH cannot be fulfilled. Furthermore we will see numerical results indicating that the ETH indeed does hold in the case of the XX-model.

3 Spin systems and fermionic models

This section gives a brief introduction to spin systems and fermionic models and the tools used in the study of the models in this thesis. It also sets up most of the notation that is later used. Spin-1/2 systems are probably the most widely studied models in theoretical physics. One of the reasons is that every spin is a two-level system. Therefore they are structurally the simplest models that can have excitations. This sometimes admits analytical solutions, which are in general very rare. At the same time, even in the case of one-dimensional models, they can already show a rich variety of phenomena. Thus they constitute a good testing ground for physical theories. Recently, as a natural example of *qubits*, they received an additional amount of attention in the study of quantum information and quantum computation.

Fermionic systems are a natural counterpart to spin systems. Due to the Pauli-principle a fermionic site is also a two-level systems and in one dimension it is possible to map a fermionic system to a spin system and vice-versa. In some cases this allows a much simpler treatment.

3.1 Spin systems

A system of spins is generally thought of as a graph $G = (V, E)$ with vertex set V and edge set E. Every vertex (or site) of the graph has a local Hilbert-space $\mathcal{H}_2 \simeq \mathbb{C}^2$ attached to it which represents a spin at this site. The simplest example of such a system is a linear chain of N spins with a total Hilbert-space dimension 2^N. The Hamiltonian of the system is often considered to be of the form $H = \sum_j h_j$ where every term h_j only acts on k spins at once. This property is usually referred to as k-locality. A model with only next-neighbor and on-site interactions is therefore 2-local. A particular example of such a system is the XY-model [23] with Hamiltonian

$$H = -\frac{1}{2} \sum_{<i,j>} \left(\frac{1+\gamma}{4} X_i X_j + \frac{1-\gamma}{4} Y_i Y_j \right) - \frac{\lambda}{2} \sum_{j=1}^{N} Z_j, \tag{8}$$

where $< i, j >$ denotes the sum over nearest neighbors, γ is called the anisotropy parameter and λ is a magnetic field in z-direction. The operators X_j, Y_j and Z_j denote the Pauli

operators σ_x, σ_y and σ_z acting only on the j-th spin. Hence

$$X_j = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \sigma_x \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}$$

and Y_j, Z_j analogously. In the isotropic case $\gamma = 0$ the model is called XX-model.

3.2 Fermionic models

A fermionic system is usually described as a collection of N sites. A site is called occupied or filled if there is a fermion at the site and empty otherwise. The Hamiltonian of such a system is written in second quantization as a sum of annihilation and creation operators $f_j, f_j^\dagger$ that obey the canonical anti-commutation rules

$$\left\{ f_i^\dagger, f_j \right\} = \delta_{i,j}, \quad \left\{ f_i^\dagger, f_j^\dagger \right\} = 0, \quad \{ f_i, f_j \} = 0,$$

where $\{A, B\} = AB + BA$. Due to the Pauli-principle there can be either one or zero fermions at each site, thus $f_j^2 = {f_j^\dagger}^2 = 0$. A system described by a Hamiltonian that is quadratic in the annihilation and creation operators, i.e. of the form

$$H = \frac{1}{2} \sum_{i,j=1}^{N} \left(f_j^\dagger A_{i,j} f_j - f_i A_{i,j} f_j^\dagger + f_i B_{i,j} f_j - f_i^\dagger B_{i,j} f_j^\dagger \right), \tag{9}$$

with real matrices A, B, is called *quasi free* [24]. For H to be Hermitian it is necessary that $A = A^\top$ and $B = -B^\top$.

It is always possible to write a quadratic Hamiltonian H in the form

$$H = \sum_k \lambda_k \eta_k^\dagger \eta_k,$$

where the $\eta_k^\dagger, \eta_k$ are again fermionic creation and annihilation operators, respectively, which in this case are usually referred to as *modes* instead of sites. An eigenstate of such an Hamiltonian can be written in the *occupation number basis* as

$$|k_1, \ldots, k_N\rangle, \quad k_j \in \{0, 1\},$$

where $k_j = 1$ if the j-th mode is occupied and $k_j = 0$ if it is empty.

As a mode can either be filled with one fermion, or be empty, a system of N fermionic sites is described by the tensor-product of N Hilbert-spaces that are each isomorphic to $\mathbb{C}^2$. The total Hilbert-space therefore has dimension 2^N.

When dealing with fermionic systems it is often useful to introduce so-called Majorana-operators $x_j = \frac{1}{\sqrt{2}} \left(f_j^\dagger + f_j \right), p_j = \frac{-\mathrm{i}}{\sqrt{2}} \left(f_j^\dagger - f_j \right)$ as coordinates. Note that they are Hermitian. With these at hand, the Hamiltonian of a fermionic system can also be written as a sum of Majorana-operators. Let $\omega = (x_1, p_1, \ldots, x_N, p_N)^\top$, such that $x_j = \omega_{2j-1}, p_j = \omega_{2j}$. A quasi-free system can be written as,

$$H = \mathrm{i} \omega^\top h \omega,$$

with $h \in \mathbb{R}^{2N \times 2N}$ and $h = -h^\top$. The Majorana-operators as defined above fulfill the anti-commutation relations

$$\{\omega_i, \omega_j\} = \delta_{i,j},$$

which are preserved by orthogonal transformations.

3.2.1 Covariance matrix

For fermionic systems the covariance matrix γ is defined as the matrix with elements

$$\gamma_{i,j} = \mathrm{i}\langle[\omega_i, \omega_j]\rangle = 2\mathrm{i}\langle\omega_i\omega_j\rangle - \mathrm{i}\delta_{i,j}. \tag{10}$$

Note that $\gamma = -\gamma^\top$. Eigenstates, ground states, and Gibbs states of quasi free fermionic systems are Gaussian [25, 26]. Thus they are completely described by their first and second moments. For fermionic systems the first moments always vanish as the Hamiltonian has to preserve the total number of fermions due to the super-selection rule of the parity of fermions. Hence, the eigenstates, ground states and the Gibbs state of a fermionic quasi-free system are completely described by their covariance matrices.

As the covariance matrix γ and the matrix h that defines the coupling in the Hamiltonian are skew-symmetric $2N \times 2N$ matrices they can be brought into a normal-form by an orthogonal transformation R,

$$R\gamma R^\top = \bigoplus_j \mu_j \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \bigoplus_j \mu_j J_2,$$

where the real numbers μ_j are given by the imaginary part of the eigenvalues of γ. If γ is a fermionic covariance matrix $\mu_j \in [-1, 1]$.

The energy expectation value of a state can directly be computed from the covariance matrix and h:

Lemma 1 (Energy expectation value) *Let $H = \mathrm{i}\omega^\top h\omega$ as before and let ρ be a state. Then the expectation value of H is given by*

$$\langle H\rangle = \frac{1}{2}\mathsf{Tr}\left(\gamma^\top h\right) = -\frac{1}{2}\mathsf{Tr}\left(\gamma h\right).$$

Proof The proof is straightforward calculation:

$$\langle H\rangle = \mathsf{Tr}\left(\rho H\right) = \mathsf{Tr}\left(\rho\mathrm{i}\omega^\top h\omega\right)$$
$$= \sum_{i,j}\mathsf{Tr}\left(\rho h_{i,j}\mathrm{i}\omega_i\omega_j\right) = \sum_{i,j}\frac{1}{2}h_{i,j}\gamma_{i,j} = \frac{1}{2}\mathsf{Tr}\left(\gamma^\top h\right),$$

where we have used that $h_{i,i} = 0$ because $h = -h^\top$.   ∎

As we are interested in thermalization the covariance matrix of a Gibbs state will be very important later. Given the Hamiltonian in normal-form it is particularly easy to calculate the covariance matrix of a Gibbs state as shown by the following Lemma.

Lemma 2 (Covariance Matrix of Gibbs state) *Let the Hamiltonian of a free fermionic system be given by*

$$H = \mathrm{i}\omega^\top h\omega,$$

with $\omega = (\omega_1, \ldots, \omega_{2N})^\top$ and $h = \oplus_j \epsilon_j J_2$. Then the covariance matrix of the Gibbs state $\rho_{\mathsf{Gibbs}} = Z^{-1}\exp(-\beta H)$ is

$$\gamma = -\bigoplus_{j=1}^{N} \tanh\left(\epsilon_j\beta\right) J_2. \tag{11}$$

PROOF Using the commutation relations for the Majorana-operators the Hamiltonian can be written as

$$H = \sum_j \epsilon_j 2\mathrm{i}\omega_{2j-1}\omega_{2j}.$$

Note that all terms in the sum commute and $(2\mathrm{i}\omega_{2j-1}\omega_{2j})^2 = \mathbb{1}$. It therefore follows by lemma 3 (see section 4) that

$$e^{-\beta H} = \prod_j \left(\cosh(\epsilon_j\beta)\mathbb{1} - \sinh(\epsilon_j\beta)2\mathrm{i}\omega_{2j-1}\omega_{2j}\right).$$

The Gibbs state therefore reads

$$\rho_{\mathsf{Gibbs}} = \prod_j \left(\frac{1}{2}\mathbb{1} - \frac{1}{2}\tanh(\epsilon_j\beta)2\mathrm{i}\omega_{2j-1}\omega_{2j}\right).$$

Looking at the anti-commutation relations for the Majorana-operators and noting that Majorana-operators are traceless it is clear that

$$\gamma_{i,j} = 2\mathrm{i}\mathrm{Tr}\left(\omega_i\omega_j \prod_l \left(\frac{1}{2}\mathbb{1} - \frac{1}{2}\tanh(\epsilon_l\beta)2\mathrm{i}\omega_{2l-1}\omega_{2l}\right)\right) - \mathrm{i}\delta_{i,j}$$

$$= \begin{cases} -\tanh\left(\epsilon_l\beta\right) & \text{if } i = 2l-1, j = 2l \\ +\tanh\left(\epsilon_l\beta\right) & \text{if } i = 2l, j = 2l-1 \\ 0 & \text{otherwise} \end{cases}.$$

Hence

$$\gamma = -\bigoplus_{j=1}^{N} \tanh\left(\epsilon_j\beta\right) J_2. \qquad \blacksquare$$

Corollary 1 *Note that $J_2 = \mathrm{i}w\sigma_z w^\dagger$ with*

$$w = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ \mathrm{i} & -\mathrm{i} \end{pmatrix}.$$

Therefore h can be brought into diagonal-form by first bringing it into the normal-form and then applying the transformation w:

$$h = Rh^{\mathsf{n.f.}}R^\top = R\bigoplus_{j=1}^{N}\epsilon_j J_2 R^\top$$

$$= R\bigoplus_{j=1}^{N}\mathrm{i}\epsilon_j w\sigma_z w^\dagger R^\top$$

$$= R\left(\bigoplus_{j=1}^{N}w\right)\left(\bigoplus_{j=1}^{N}\mathrm{i}\epsilon_j\sigma_z\right)\left(\bigoplus_{j=1}^{N}w^\dagger\right)R^\top.$$

Together with the facts $\tan(\mathrm{i}x) = \mathrm{i}\tanh(x)$ and $\tanh(-x) = -\tanh(x)$ this shows

$$\gamma^{\mathsf{Gibbs}} = -\tan\left(\beta h\right). \qquad \square$$

3.2.2 Jordan-Wigner transformation

A system composed of N spins and a system of N fermionic sites both have Hilbert-spaces $\mathcal{H} \simeq \left(\mathbb{C}^2\right)^{\otimes N}$ of dimension 2^N. It is therefore tempting to identify an occupied fermionic site with a spin-up or spin-down state in a spin model. Indeed there exists an isomorphism between one-dimensional spin-models and one-dimensional fermionic models, the Jordan-Wigner transformation [27]. Given a spin system it is defined by setting

$$Z_i = 1 - 2f_i^\dagger f_i$$

$$S_i^+ = \prod_{k=1}^{i-1} \left(1 - 2f_k^\dagger f_k\right) f_i^\dagger$$

$$S_i^- = \prod_{k=1}^{i-1} \left(1 - 2f_k^\dagger f_k\right) f_i,$$

where $S_i^\pm = \left(X_i \pm iY_i\right)/2$. A spin-down state in the spin-model is then equivalent to an occupied site in the fermionic model. Note that due to the factors $\prod_{k=1}^{i-1} \left(1 - 2f_k^\dagger f_k\right)$ this transformation does in general not preserve locality.

4 First model

Let us now turn to the first model. This model is primarily used to study whether it is really necessary to consider all conserved quantities when calculating the equilibrium state of a subsystem or if it is sufficient to consider only the local conserved quantities. I will also discuss if the Eigenstate Thermalization Hypothesis holds.

The model is a linear chain of N spins. We first define the Hermitian operators

$$H = \sum_{i=1}^{N} \lambda_i Z_i,$$

and

$$V = \sum_{i=1}^{N} X_i X_{i+1},$$

where we assume periodic boundary conditions, such that $X_N X_{N+1} = X_N X_1$. The operator H can be regarded as a Hamiltonian of N spins without any interaction but with a local magnetic field in z-direction of strength λ_i. The parameters λ_i are thought of as random numbers chosen from a Gaussian distribution with mean λ and variance σ^2, where the variance is considered to be small. The important point is, that it destroys any degeneracies of the Hamiltonian H. Our model Hamiltonian $\mathfrak{H}$ is now given by the conjugation of H with $U = \exp\left(iV\tau\right)$:

$$\mathfrak{H} = UHU^\dagger = e^{iV\tau} H e^{-iV\tau}$$

$$= \sum_{i=1}^{N} e^{iV\tau} \lambda_i Z_i e^{-iV\tau}.$$

The resulting Hamiltonian still has the same spectrum as H and one can think of it as a rotated version of H. I will sometimes refer to it as the rotated Hamiltonian. From the general arguments in ref. [10] it can be expected that such a system thermalizes. If we write a local spin-up state as $|1\rangle = (1,0)^\top$ and the spin-down state as $|0\rangle = (0,1)^\top$ the

eigenstates of H are

$$|k_1, \ldots, k_N\rangle = |k_1\rangle \otimes \ldots \otimes |k_N\rangle, \quad k_j \in \{0, 1\}$$

and therefore the set of eigenstates of $\mathfrak{H}$ is

$$\{e^{iV\tau} |k_1, \ldots, k_N\rangle \mid k_j \in \{0, 1\}\}. \tag{12}$$

In the following it will often be necessary to explicitly calculate how operators like e^{aA}, where a is a real or complex number and A an operator, act on states or other operators. The following Lemma will often be useful in these calculations.

Lemma 3 *Let A be any operator with the property that A^2 is proportional to the identity. We set $A^2 = \alpha\mathbb{1}$ with $\alpha \in \mathbb{R}$. Let $a \in \mathbb{C}$. Then*

$$e^{aA} = \left[\cosh(\mathrm{Re}(a)\sqrt{\alpha})\mathbb{1} + \frac{1}{\sqrt{\alpha}} \sinh(\mathrm{Re}(a)\sqrt{\alpha})A\right] \left[\cos(\mathrm{Im}(a)\sqrt{\alpha})\mathbb{1} + \frac{i}{\sqrt{\alpha}} \sin(\mathrm{Im}(a)\sqrt{\alpha})A\right],$$
$$\tag{13}$$

where $\mathrm{Re}(\cdot)$ and $\mathrm{Im}(\cdot)$ denote the real- and imaginary part, respectively.

PROOF As $e^{(\mathrm{Re}(a)+i\mathrm{Im}(a))A} = e^{\mathrm{Re}(a)A}e^{i\mathrm{Im}(a)A}$ it suffices to treat the real and imaginary part of a separately and then multiply them. So let $a \in \mathbb{R}$. By writing out the series expansion of e^{aA} one gets

$$e^{aA} = \sum_{k=0}^{\infty} \frac{a^{2k}A^{2k}}{2k!}\mathbb{1} + \sum_{k=0}^{\infty} \frac{a^{2k+1}A^{2k}}{(2k+1)!}A$$

$$= \sum_{k=0}^{\infty} \frac{a^{2k}\sqrt{\alpha}^{2k}}{2k!}\mathbb{1} + \frac{1}{\sqrt{\alpha}} \sum_{k=0}^{\infty} \frac{a^{2k+1}\sqrt{\alpha}^{2k+1}}{(2k+1)!}A$$

$$= \cosh(a\sqrt{\alpha})\mathbb{1} + \frac{1}{\sqrt{\alpha}} \sinh(a\sqrt{\alpha})A.$$

The case when a is purely imaginary then follows from $\sinh(ix) = i\sin(x)$ and $\cosh(ix) = \cos(x)$.

∎

Locality of the rotated Hamiltonian The rotation of H by U changes the locality of H. To see this we calculate how conjugation by U acts on one term Z_J. As all the operators X_j, X_k commute we can write U as

$$U = \prod_j e^{i\tau X_j X_{j+1}} = \prod_j u_j,$$

where each u_j is unitary and has support on sites j and $j+1$. As $u_j u_j^\dagger = \mathbb{1}$ it follows that

$$UZ_jU^\dagger = u_{j-1}u_j Z_j u_{j-1}^\dagger u_j^\dagger,$$

which is a 3-local operator that acts on the sites $j-1, j, j+1$.

4.1 Conserved quantities

We have seen above that the going from the system described by H to the model is basically done by "conjugating everything by $U = \exp(iV\tau)$". Is this also true for the conserved quantities? Let o be the set of operators conserved by H,

$$o = \{A \mid [H, A] = 0\},$$

and O the set of operators conserved by the model Hamiltonian,

$$O = \{B \mid [UHU^\dagger, B] = 0\}.$$

We ask if $O = UoU^\dagger = \{UAU^\dagger \mid [H, A] = 0\}$. Let $B \in O$. Then $U^\dagger [UHU^\dagger, B] U = [H, U^\dagger BU] = 0$. So $U^\dagger BU \in o$, which just means that every B can be written as the conjugation of an A. By an analog argument it is possible to show that $UAU^\dagger \in O$ for all $A \in o$, so $UoU^\dagger = O$.

   To find all the conserved quantities of the model it therefore suffices to find all quantities conserved by H and conjugate. Note however again that conjugation does not preserve locality.

4.1.1 Projectors of unrotated Hamiltonian

Let P_n denote the projector onto the eigenspace of the n-th eigenvalue E_n of H. It has the form

$$|k_1, \ldots, k_N\rangle\langle k_1, \ldots, k_N| = |k_1\rangle\langle k_1| \otimes \cdots \otimes |k_N\rangle\langle k_N|,$$

where of course $k_1, \ldots, k_N \in \{0, 1\}$. Depending on the value of k_j the projector onto the subspace of the j-th spin in this state can be written as

$$\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes |k_j\rangle\langle k_j| \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} = \frac{\mathbb{1} \pm Z_j}{2},$$

with $-$ in the case $k_j = 0$ and $+$ if $k_j = 1$. Therefore P_n has the form

$$P_n = \frac{1}{2^N} (\mathbb{1} \pm Z_1) \cdots (\mathbb{1} \pm Z_N).$$

As the Hamiltonian H is given by

$$H = \sum_n E_n P_n,$$

it is clear that every such projector is a conserved quantity. Note that it is not a local conserved quantity.

   As the Hamiltonian is non-degenerate the 2^N projectors P_n form a linear basis for the conserved quantities. The relation $P_{n'}P_n = P_n \delta_{n.n'}$ implies that they are also algebraically independent and clearly commute.

4.1.2 Strings of Pauli-Z-operators

All the projectors P_n are products of N terms of the form $\frac{\mathbb{1} \pm Z_j}{2}$. Multiplying out all the factors yields a sum of the form

$$\sum_{\Lambda \subseteq \Omega} \pm 2^{-|\Lambda|} Z_\Lambda,$$

where $\Omega = \{1, \ldots, N\}$ is the set of all spins and $Z_\Lambda = \prod_{j \in \Lambda} Z_j$ is an operator with support only on Λ. The sign in each term depends on the state associated with the projector.

All 2^N operators Z_Λ clearly commute with H individually and commute pairwise. Every projector is a linear combination of all Z_Λ and therefore every conserved quantity can be written as a linear combination of the operators Z_Λ. Note that while the Z_Λ are linearly independent they are not algebraically independent as

$$Z_{\Lambda_1} Z_{\Lambda_2} = Z_{\Lambda_1 \triangle \Lambda_2},$$

where $\Lambda_1 \triangle \Lambda_2$ is the symmetric difference $(\Lambda_1/\Lambda_2) \cup (\Lambda_2/\Lambda_1)$. Also while the projectors P_n are global operators the Z_Λ are local operators with support of size $|\Lambda|$ and each set

$$\mathcal{Z}_\Gamma = \{Z_\Lambda \mid \Lambda \subseteq \Gamma\}$$

is a basis for the local conserved quantities on the subsystems Γ.

4.1.3 Time-average of states

If a system thermalizes then it has to equilibrate, and if it equilibrates it has to equilibrate to its time-average. It is therefore important to know how time-averages behave in the model. We will now see how the time average of a state ρ relates to the time-average of ρ conjugated by the unitary operator $U = \exp{(iV\tau)}$. To do this we write H as

$$H = \sum_n E_n P_n,$$

where P_n are the projectors onto the subspaces with energy E_n. The time-average of a state ρ is

$$\langle \rho \rangle_t = \lim_{T \to \infty} \frac{1}{T} \int_0^T \sum_{m,n} e^{i(E_m - E_n)t} P_n \rho P_m \, \mathrm{d}t \tag{14}$$

$$= \sum_n P_n \rho P_n. \tag{15}$$

The time-average of the rotated state $U\rho U^\dagger$ is

$$\langle U\rho U^\dagger \rangle_t = \lim_{T \to \infty} \frac{1}{T} \int_0^T e^{-iUHU^\dagger t} U\rho U^\dagger e^{iUHU^\dagger t} \, \mathrm{d}t$$

$$= \lim_{T \to \infty} \frac{1}{T} \int_0^T U e^{-iHt} U^\dagger U\rho U^\dagger U e^{iHt} U^\dagger \, \mathrm{d}t$$

$$= U \left(\lim_{T \to \infty} \frac{1}{T} \int_0^T e^{-iHt} \rho \, \mathrm{d}t \right) U^\dagger = U \langle \rho \rangle_t U^\dagger.$$

So it does not matter if time-averaging or conjugation by U is done first.

4.1.4 Maximum entropy or equilibrium state

Let us proceed to calculate the maximum entropy state for any given expectation values of the set of conserved quantities. Recall that the maximum entropy state is given by an exponential of a linear combination of all conserved quantities. As $\exp(UAU^\dagger) = U\exp(A)U^\dagger$ we can first calculate the maximum entropy state for the unrotated Hamiltonian and then conjugate to go over to the rotated Hamiltonian. We therefore begin with the maximum entropy state of the unrotated Hamiltonian.

As later only local observables are of interest, it is convenient to take the set $\mathcal{Z} = \{Z_\Lambda\}_{\Lambda \subseteq \Omega}$ as linear basis for the conserved quantities. Note that all $Z_\Lambda \in \mathcal{Z}$ commute pairwise. Let

us introduce an index set Γ that counts the $2^N = 2^{|\Omega|}$ different subsets of $\Omega = \{1, \ldots, N\}$. Then the set $\{\Lambda_k\}_{k \in \Gamma}$ is the set of all subsets of Ω. The maximum entropy state, or GGE, is given by

$$\omega \propto \exp\left(-\sum_{k \in \Gamma} \beta_k Z_{\Lambda_k}\right)$$
$$= \prod_{k \in \Gamma} \exp\left(-\beta_k Z_{\Lambda_k}\right),$$

because all the Z_{Λ_k} commute. By lemma 3 it follows that

$$\omega \propto \prod_{k \in \Gamma} \left(\cosh\left(\beta_k\right) \mathbb{1} - \sinh\left(\beta_k\right) Z_{\Lambda_k}\right)$$
$$= \sum_{\Xi \subseteq \Gamma} \prod_{j \in \Xi^c} \cosh\left(\beta_j\right) \prod_{k \in \Xi} (-1) \sinh\left(\beta_k\right) Z_{\Lambda_k},$$

where $\Xi^c = \Gamma/\Xi$. Note that $\prod_{k \in \Xi} Z_{\Lambda_k} = Z_\Lambda$ for some $\Lambda \subseteq \Omega$. Collecting all terms where the product $\prod_{k \in \Xi} Z_{\Lambda_k}$ yields the same Z_Λ we can write the state as

$$\omega = \sum_{\Lambda \subseteq \Omega, \Lambda \neq \emptyset} c_\Lambda Z_\Lambda + c_\emptyset \mathbb{1}.$$

Normalization requires that $c_\emptyset = 2^{-N}$. All the expectation values $\langle Z_{\Lambda'}\rangle$ are given by

$$\langle Z_{\Lambda'}\rangle = \text{Tr}\left(Z_{\Lambda'}\omega\right) = \sum_\Lambda \text{Tr}\left(c_\Lambda Z_{\Lambda \triangle \Lambda'}\right) + 2^{-N}\text{Tr}\left(Z_{\Lambda'}\right)$$
$$= 2^N c_{\Lambda'},$$

as $\text{Tr}\left(\sigma_z\right) = 0$ and $\text{Tr}\left(A \otimes B\right) = \text{Tr}\left(A\right)\text{Tr}\left(B\right)$. Hence we have

$$c_\Lambda = \frac{\langle Z_\Lambda\rangle}{2^N}.$$

Note again that the expectation values $\langle Z_\Lambda\rangle$ are fixed by the initial state.

What happens if we only fix the expectation value of local conserved quantities on some subsystem Σ? Let Γ_S be the index set that counts the different regions Λ_k inside $\Sigma \subseteq \Omega$. Then we get as total state with maximum entropy

$$\sigma = \sum_{\Lambda \subseteq \Sigma, \Lambda \neq \emptyset} c_\Lambda^S Z_\Lambda + c_\emptyset^S \mathbb{1},$$

by the same calculation as above. As we require that $\langle Z_\Lambda\rangle_\omega = \langle Z_\Lambda\rangle_\sigma$ for all $\Lambda \subseteq \Sigma$, it follows that $c_\Lambda^S = c_\Lambda$ for all $\Lambda \subseteq \Sigma$. The reductions of σ and ω to Σ are then

$$\omega_\Sigma = \text{Tr}_{\Omega/\Sigma}\left(\sum_{\Lambda \subseteq \Omega, \Lambda \neq \emptyset} c_\Lambda Z_\Lambda\right) + \text{Tr}_{\Omega/\Sigma}\left(c_\emptyset \mathbb{1}\right),$$
$$= 2^{|\Omega/\Sigma|}\left(\sum_{\Lambda \subseteq \Sigma, \Lambda \neq \emptyset} c_\Lambda^S Z_\Lambda + c_\emptyset^S \mathbb{1}\right)$$
$$\sigma_\Sigma = 2^{|\Omega/\Sigma|}\left(\sum_{\Lambda \subseteq \Sigma, \Lambda \neq \emptyset} c_\Lambda^S Z_\Lambda + c_\emptyset^S \mathbb{1}\right),$$

where the relations $\mathrm{Tr}\,(\sigma_z) = 0$ and $\mathrm{Tr}\,(A \otimes B) = \mathrm{Tr}\,(A)\,\mathrm{Tr}\,(B)$ have been used. The operators Z_Λ and $\mathbb{1}$ are now, of course, only defined on the set Σ instead of Ω. So the two states are the same.

With the results for the unrotated Hamiltonian at hand it is now possible to calculate the maximum entropy for the rotated Hamiltonian. As discussed in the beginning of this section this simply done by conjugating ω by U. Thus the state of maximum entropy for the rotated Hamiltonian is

$$U\omega U^\dagger = \sum_{\Lambda \subseteq \Omega, \Lambda \neq \emptyset} c'_\Lambda U Z_\Lambda U^\dagger + c_\emptyset \mathbb{1}, \tag{16}$$

where $c'_\Lambda = 2^{-N}\langle U Z_\Lambda U^\dagger \rangle$.

The difference to the unrotated case lies in the fact that the rotation by U induces interactions between neighboring sites and therefore in general $\mathrm{Tr}_{\Lambda_2}\left(U Z_{\Lambda_1} Z_{\Lambda_2} U^\dagger\right) \neq 0$, even when Λ_1 and Λ_2 are disjoint.

Ultimately we are interested in the reduction of $U\omega U^\dagger$ to some small subsystem. To calculate the reduction it is necessary to study the unitary U more carefully. At first, we can write out U more explicitly. Note that $(X_j X_{j+1})^2 = \mathbb{1}$, it then follows, again by lemma 3, that

$$U = \prod_{j=1}^{N} \exp\left(\mathrm{i}\tau X_j X_{j+1}\right) = \prod_{j=1}^{N} \left(\cos(\tau)\mathbb{1} + \mathrm{i}\sin(\tau)X_j X_{j+1}\right)$$

$$= \sum_{\substack{\Gamma \subseteq \Omega \\ |\Gamma|\,\mathrm{even} \\ \Gamma \neq \emptyset}} u_\Gamma X_\Gamma + \cos(\tau)^N \mathbb{1},$$

where u_Γ are of the form $\mathrm{i}^j \sin(\tau)^j \cos(\tau)^k$ and j, k depend on the region Γ with $j + k = N$. Now consider one term $U Z_\Lambda U^\dagger$ in eq. 16. We define again the union of a set of M consecutive sites $\Lambda = \{k, \ldots, k + M\}$ with its boundary to be the set $\partial\Lambda = \{k - 1, \ldots, k + M + 1\}$. General sets are disjoint unions of sets of a number of consecutive sites. The boundary set is then defined as the union of all the boundary sets of the disjoint subsets. Furthermore we define the unitary matrices on sets $\Lambda \neq \Omega$

$$U_\Lambda = \prod_{\substack{j \\ j, j+1 \in \partial\Lambda}} \exp\left(\mathrm{i}\tau X_j X_{j+1}\right) = \sum_{\substack{\Gamma \subseteq \partial\Lambda \\ |\Gamma|\,\mathrm{even}}} u_\Gamma X_\Gamma,$$

where now the powers j, k in u_Γ have to sum up to $|\Lambda| + 1$. Then U can be written as

$$U = U_\Lambda U_{\Omega/\partial\Lambda}$$

and as $U_\Lambda^\dagger U_\Lambda = U_\Lambda U_\Lambda^\dagger = \mathbb{1}$ we have

$$U Z_\Lambda U^\dagger = U_{\Omega/\partial\Lambda} U_\Lambda Z_\Lambda U_\Lambda^\dagger U_{\Omega/\partial\Lambda}^\dagger = U_\Lambda Z_\Lambda U_\Lambda^\dagger$$

$$= \sum_{\substack{\Gamma \subseteq \partial\Lambda \\ |\Gamma|\,\mathrm{even}}} \sum_{\substack{\Gamma' \subseteq \partial\Lambda \\ |\Gamma'|\,\mathrm{even}}} u_\Gamma X_\Gamma Z_\Lambda \bar{u}_{\Gamma'} X_{\Gamma'}$$

$$= \sum_{\substack{\Gamma \subseteq \partial\Lambda \\ |\Gamma|\,\mathrm{even}}} \sum_{\substack{\Gamma' \subseteq \partial\Lambda \\ |\Gamma'|\,\mathrm{even}}} u_\Gamma \bar{u}_{\Gamma'} X_\Gamma Z_\Lambda X_{\Gamma'}. \tag{17}$$

Let us now observe what happens to the operators Z_Λ and $X_\Gamma Z_\Lambda X_{\Gamma'}$ if we trace out everything but a region Σ of our system. Recall that the Pauli-operators fulfill

$$\sigma_i \sigma_j = \delta_{i,j} + \mathrm{i} \sum_k \epsilon_{i,j,k} \sigma_k,$$

where $\epsilon_{i,j,k}$ is the Levi-Civita tensor. Also note that the Pauli-operators are traceless. This implies that all the operators vanish in the case that $\Lambda \not\subseteq \Sigma$. If $\Lambda \subseteq \Sigma$ there are two case: $\partial\Lambda \subseteq \Sigma$ and $\partial\Lambda \cap (\Omega/\Sigma) \neq \emptyset$. In the first case we get

$$\mathrm{Tr}_\Sigma \left(X_\Gamma Z_\Lambda X_{\Gamma'} \right) = 2^{|\Omega/\Sigma|} X_\Gamma Z_\Lambda X_{\Gamma'},$$

$$\mathrm{Tr}_\Sigma \left(Z_\Lambda \right) = 2^{|\Omega/\Sigma|} Z_\Lambda,$$

where, of course, $X_\Gamma, X_{\Gamma'}, Z_\Lambda$ are now only defined on Σ. We therefore have, in this case, $\mathrm{Tr}_\Sigma \left(U_\Lambda Z_\Lambda U_\Lambda^\dagger \right) = 2^{|\Omega/\Sigma|} U_\Lambda Z_\Lambda U_\Lambda^\dagger$. In the case $\partial\Lambda \cap (\Omega/\Sigma) \neq \emptyset$ the sum in eq. 17 reduces to

$$\sum_{\substack{\Gamma \subseteq \Sigma \cap \partial\Lambda \\ |\Gamma| \text{ even}}} \sum_{\substack{\Gamma' \subseteq \Sigma \cap \partial\Lambda \\ |\Gamma'| \text{ even}}} u_\Gamma \bar{u}_{\Gamma'} X_\Gamma Z_\Lambda X_{\Gamma'}. \tag{18}$$

It is therefore possible to write the reduced state of the thermal state as

$$\sigma_\Sigma = 2^{|\Omega/\Sigma|} \left[\sum_{\substack{\partial\Lambda \subseteq \Sigma \\ \Lambda \neq \emptyset}} c_\Lambda U_\Lambda Z_\Lambda U_\Lambda^\dagger + c_\emptyset \mathbb{1} \right] + \mathrm{Tr}_\Sigma \left(R_\Sigma \right),$$

with

$$R_\Sigma = \sum_{\substack{\Lambda \subseteq \Sigma \\ \partial\Lambda \cap (\Omega/\Sigma) \neq \emptyset}} c_\Lambda \sum_{\substack{\Gamma \subseteq \Sigma \cap \partial\Lambda \\ |\Gamma| \text{ even}}} \sum_{\substack{\Gamma' \subseteq \Sigma \cap \partial\Lambda \\ |\Gamma'| \text{ even}}} u_\Gamma \bar{u}_{\Gamma'} X_\Gamma Z_\Lambda X_{\Gamma'}.$$

The first term is the same state as we would have gotten if we had only fixed the expectation values of all operators $U Z_\Lambda U^\dagger$ with $\partial\Lambda \subseteq \Sigma$ and calculated the maximum entropy state. The second term is a residual term. The residual term only contains contributions from conserved quantities that have support on the boundary of Σ. Therefore we have shown that indeed only the expectation values of the conserved quantities on a subsystem together with its boundary are needed to compute the equilibrium state of the subsystem.

Note that this result is technically mainly caused by the fact that the interactions are given by tensor products of traceless operators, namely the Pauli operators, and the identity.

4.2 ETH and fermionic picture

The second purpose of the model is to check whether the Eigenstate Thermalization Hypothesis holds for this model. To do this we will have to calculate reductions of eigenstates of the Hamiltonian. In the case of free fermions this can easily be done as the reduced state of a quasi free state is fully determined by its covariance matrix. The covariance matrix of a reduced state is given by the subsystem's part of the original covariance matrix. For eigenstates of quasi free systems the covariance matrix is easy to calculate. As shown by lemma 2 the covariance matrix of a Gibbs state is also easy to calculate. The strategy to check whether the ETH holds will therefore be the following. First, the model is transformed to a fermionic model using the Jordan-Wigner transformation, hoping that it turns out to be a quasi free model. We will find out that it does turn out to be free.

Then the covariance matrices of eigenstates are calculated. Finally, we see if it is possible that eigenstates of similar energy have the same reduced states.

Performing the Jordan-Wigner transformation as discussed in section 3.2.2 yields

$$H \mapsto \tilde{H} = \sum_{j=1}^{N} \lambda_j \left(1 - 2 f_j^\dagger f_j \right) \tag{19}$$

$$= \sum_{j=1}^{N} \lambda_j \, 2\mathrm{i}\omega_{2j-1}\omega_{2j}, \tag{20}$$

$$V \mapsto \tilde{V} = \sum_{j=1}^{N} \mathrm{i}\omega_{2j}\omega_{2j+1}, \tag{21}$$

where ω_j denote the Majorana-operators. Note that the locality of the operators is preserved in this case.

Using lemma 3 and the commutation relation for Majorana-operators one can directly compute the Hamiltonian of the rotated model to be

$$\tilde{\mathfrak{H}} = \sum_{j=1}^{N} \lambda_j \exp\left(\mathrm{i}\tilde{V}\tau\right) \omega_{2j-1}\omega_{2j} \exp\left(-\mathrm{i}\tilde{V}\tau\right) \tag{22}$$

$$= 2\mathrm{i}\lambda\omega^\top S\Lambda S^\top \omega, \tag{23}$$

where Λ has the form

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix} \tag{24}$$

and $S^\top$ is the orthogonal transformation that reorders the entries in ω in the following way:

$$(\omega_1, \omega_2, \ldots, \omega_{2N-1}, \omega_{2N}) \rightarrow (\omega_1, \ldots, \omega_{2N-1}, \omega_2, \ldots, \omega_{2N}).$$

The Matrices A and B are given by

$$A = \alpha \begin{pmatrix}
0 & 1 & 0 & \cdots & 0 & -1 \\
-1 & 0 & 1 & 0 & \ddots & 0 \\
0 & -1 & 0 & \ddots & 0 & \vdots \\
\vdots & 0 & \ddots & 0 & 1 & 0 \\
0 & \ddots & 0 & -1 & 0 & 1 \\
1 & 0 & \cdots & 0 & -1 & 0
\end{pmatrix}$$

$$B = \beta\mathbb{1} + \gamma \begin{pmatrix}
0 & 0 & 1 & 0 & \cdots & 0 & 1 & 0 \\
0 & & 0 & \ddots & 0 & & 0 & 1 \\
1 & 0 & & \ddots & \ddots & \ddots & & 0 \\
0 & \ddots & \ddots & & & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & & & \ddots & 0 \\
0 & & \ddots & \ddots & \ddots & & 0 & 1 \\
1 & 0 & & \ddots & \ddots & 0 & & 0 \\
0 & 1 & 0 & \cdots & 0 & 1 & 0 & 0
\end{pmatrix},$$

where α, β and γ are functions of τ with $\alpha(0) = \gamma(0) = 0$ and $\beta(0) = 1$:

$$\alpha\left(\tau\right) = \cos\left(\tau\right)\sin\left(\tau\right)$$
$$\beta\left(\tau\right) = \cos\left(\tau\right)^2$$
$$\gamma\left(\tau\right) = \sin\left(\tau\right)^2.$$

Note that $A = -A^\top, B = B^\top$ and therefore $\Lambda = -\Lambda^\top$. This is necessary because $\tilde{\mathfrak{H}}$ has to be Hermitian. We see that $\tilde{\mathfrak{H}}$ is quadratic in the Majorana-operators. Therefore the model is indeed a quasi-free model.

4.2.1 Transformation of the covariance matrix

We have seen that the model is quasi free model in the fermionic picture. The next step is to calculate the covariance matrices of eigenstates. In the calculation of the equilibrium state of a subsystem in the spin picture, we saw that it was useful to first consider the unrotated model and see how going over to the rotated model influences the results. As the covariance matrices of eigenstates in the unrotated model are very easy to calculate, it would be nice if this intuition carries over to the calculation of covariance matrices. We will now see that it indeed does.

Recall that the covariance matrix γ of a fermionic system, described in Majorana-operators, in a state ρ is defined as

$$\gamma_{i,j} = 2\mathrm{i}\langle\omega_i\omega_j\rangle - \mathrm{i}\delta_{i,j},$$

with $\langle\omega_i\omega_j\rangle = \mathrm{Tr}\left(\omega_i\omega_j\rho\right)$. Suppose we know the covariance matrix for a state ρ in the unrotated system, for example an eigenstate. What is the covariance matrix of the corresponding rotated state $U\rho U^\dagger$, where now $U = \exp\left(\mathrm{i}\tilde{V}\tau\right)$? As the trace is invariant under cyclic permutation in the argument we have $\mathrm{Tr}\left(\omega_i\omega_j U\rho U^\dagger\right) = \mathrm{Tr}\left(U^\dagger\omega_i\omega_j U\rho\right)$. So instead of looking at the rotated state we can observe how conjugation by $U^\dagger$ acts on the operators $\omega_i\omega_j$. By using lemma 3 and the fact that U is a product of commuting 2-local unitary operators one then finds that the matrix elements $\gamma_{i,j}$ transform as following when going from ρ to $U\rho U^\dagger$:

$$\gamma_{i,j} \rightarrow \begin{cases} s^2\gamma_{i+1,j+1} - sc\left(\gamma_{i,j+1} + \gamma_{i+1,j}\right) + c^2\gamma_{i,j} & \text{if } i,j \text{ both even} \\ s^2\gamma_{i-1,j-1} + sc\left(\gamma_{i-1,j} + \gamma_{i,j-1}\right) + c^2\gamma_{i,j} & \text{if } i,j \text{ both odd} \\ -s^2\gamma_{i-1,j+1} + sc\left(\gamma_{i-1,j} - \gamma_{i,j+1}\right) + c^2\gamma_{i,j} & \text{if } i \text{ odd and } j \text{ even} \end{cases}, \quad (25)$$

with the short-notation $c = \cos\tau$ and $s = \sin\tau$. The case where i is even and j is odd follows from $\gamma = -\gamma^\top$. If we are interested in the covariance matrices of eigenstates of the rotated Hamiltonian, it therefore suffices to calculate that of the corresponding eigenstate of the unrotated Hamiltonian and use this transformation.

4.2.2 Covariance matrix of eigenstates

The unrotated Hamiltonian is already diagonal in its "local" representation. Each spin is uncorrelated from the others. Therefore the covariance matrix of an eigenstate,

$$|E_k\rangle = |k_1, \ldots, k_N\rangle,$$

is simply given by

$$\gamma_k = \bigoplus_{j=1}^{N}(-1)^{k_j}J_2.$$

Thus in this case $\gamma_{i,j} = 0$ if i and j are either both odd or both even. Note that the transformation eq. 25 only superposes next-neighbor entries of $\gamma_{i,j}$ in the matrix. It thereby only induces correlations between next neighbors. The covariance matrix of the rotated eigenstate $U |E_k\rangle\langle E_k| U^\dagger$ therefore only has non-zero entries on the two sidebands next to the diagonal.

4.2.3 Eigenstate Thermalization Hypothesis

If the strong ETH holds in this model, eigenstates of the total system with similar energy would have to look the same on all small enough subsystems. Recall that eigenstates of a quasi free fermionic system are completely described by their covariance matrix. This means that different eigenstates have to have different covariance matrices. The result from the preceding section, which showed that the covariance of eigenstates only have non-zero correlations between nearest neighbors, implies that the covariance matrices of two different eigenstates already have to differ on subsystems of size two. Therefore the ETH cannot hold for subsystems of size two. Note that in this case it was not even necessary to calculate the local Gibbs state.

5 XX-model

The second model is the XX-model. The XX-model is a widely studied model in quantum many-body physics. This is due to the fact that it can be solved fairly easily but still exhibits non-trivial effects like a quantum phase transition. It is therefore interesting to see if the ETH can hold in the model. Instead of showing analytically if the ETH can hold or not, we will see this using numerical experiments.

In general, a system of N spins or fermions is difficult to simulate on a classical computer because the dimension of the Hilbert-space grows exponentially with the number of particles. Hermitian operators on the Hilbert-space of N spins are in general described by 2^{2N} real numbers. Exact diagonalization is therefore not feasible in a situation where N is much bigger then 10, at least not on a "normal" computer.

We will see, however, that the XX-model goes over to a free fermionic chain under a Jordan-Wigner transformation. A free fermionic chain is completely described by the coupling matrix h, which is only a real $2N \times 2N$ matrix. Furthermore any Gibbs state is completely described by its real $2N \times 2N$ covariance matrix. Instead of matrices of dimensions $2^N \times 2^N$ we therefore only have to deal with matrices $2N \times 2N$ when dealing with quasi free systems. This makes numerical studies of quasi free systems feasible.

In section 3.1 the XX-model was introduced as a spin-model. We will now perform the Jordan-Wigner transformation, calculate the normal-form of the corresponding coupling matrix h and briefly discuss the criticality of the model. After that we will see how to calculate the covariance matrices of Gibbs states and eigenstates directly. Then the numerical experiments are described and finally the results are presented.

Under a Jordan-Wigner transformation the XX-model goes over to a free fermionic chain (see section 3.2),

$$H = \frac{1}{2} \sum_{i,j=1}^{N} \left(f_j^\dagger A_{i,j} f_j - f_i A_{i,j} f_j^\dagger + f_i B_{i,j} f_j - f_i^\dagger B_{i,j} f_j^\dagger \right),$$

with $B = 0$ and

$$A_{i,j} = \left\{ \begin{array}{ll} \lambda & \text{if } i = j \\ -\frac{1}{2} & \text{if } |i - j| = 1, \end{array} \right.$$

with periodic boundary conditions.

If we define $f = \left(f_1, \ldots, f_N, f_1^\dagger, \ldots, f_N^\dagger \right)$ we can write H as

$$H = \frac{1}{2} f^\top \begin{pmatrix} 0 & -A \\ A & 0 \end{pmatrix} f. \tag{26}$$

Let S again be the orthogonal transformation which reorders the entries of an vectors f in the way

$$\left(f_1, \ldots, f_N, f_1^\dagger, \ldots, f_N^\dagger \right) \to \left(f_1, f_1^\dagger, \ldots, f_N, f_N^\dagger \right)$$

and let W be the matrix

$$W = \bigoplus_{j=1}^N \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}.$$

Then we can write the vector of Majorana-operators as $\omega = WSf$ and accordingly $f = S^\top W^\dagger \omega$. Putting this into eq. 26 we get

$$H = \frac{1}{2} \omega^\top \bar{W} S \begin{pmatrix} 0 & -A \\ A & 0 \end{pmatrix} S^\top W^\dagger \omega.$$

Pulling out an i, we get back the usual form of a quasi free fermionic model in Majorana-operators $H = i\omega^\top h\omega$ with

$$h = \frac{1}{2i} \bar{W} S \begin{pmatrix} 0 & -A \\ A & 0 \end{pmatrix} S^\top W^\dagger.$$

The coupling matrix A is a real symmetric matrix, hence it can be diagonalized by an orthogonal transformation U. Let D be the diagonal form of A, so $A = UDU^\dagger$. We can then write H as

$$\begin{aligned}
H &= \frac{1}{2} \omega^\top \bar{W} S \begin{pmatrix} 0 & -A \\ A & 0 \end{pmatrix} S^\top W^\dagger \omega \\
&= \frac{1}{2} \omega^\top \bar{W} S \begin{pmatrix} 0 & -UDU^\top \\ UDU^\top & 0 \end{pmatrix} S^\top W^\dagger \omega \\
&= \frac{1}{2} \omega^\top \bar{W} S \left(U \oplus U \right) \begin{pmatrix} 0 & -D \\ D & 0 \end{pmatrix} \left(U^\top \oplus U^\top \right) S^\top W^\dagger \omega \\
&= \frac{1}{2} \omega^\top \bar{W} S \left(U \oplus U \right) S^\top S \begin{pmatrix} 0 & -D \\ D & 0 \end{pmatrix} S^\top S \left(U^\top \oplus U^\top \right) S^\top W^\dagger \omega. \tag{27}
\end{aligned}$$

If we denote the diagonal entries of D with $\epsilon_1, \ldots, \epsilon_N$ we get that

$$\frac{1}{2} S \begin{pmatrix} 0 & -D \\ D & 0 \end{pmatrix} S^\top = \bigoplus_{j=1}^N -\frac{1}{2} \epsilon_j \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \bigoplus_{j=1}^N -\frac{1}{2} \epsilon_j J_2 = h^{\text{n.f.}}$$

is the normal-form of h.

Criticality of the model   This model is interesting as it features a quantum phase transition in the parameter λ. This can be seen in the following way. Writing out the Hamiltonian in the original fermionic annihilation and creation operators instead of the Majorana-operators yields,

$$H = \sum_j \lambda f_j^\dagger f_j - \frac{1}{2} \sum_j \left(f_j^\dagger f_{j+1} + \text{h.c.} \right) + \text{const.},$$

where h.c. denotes the Hermitian conjugate of the preceding term and recall that we chose periodic boundary conditions. If we define new fermionic annihilation operators

$$\eta_j = \frac{1}{\sqrt{N}} \sum_k f_k e^{2\pi \frac{jk}{N}},$$

the Hamiltonian becomes diagonal in these operators, i.e.

$$H = \sum_k \lambda_k \eta_k^\dagger \eta_k + \text{const.},$$

where the real numbers λ_k are given by

$$\lambda_k = \lambda - \cos\left(\frac{2\pi k}{N}\right).$$

For $|\lambda| > 1$ the numbers λ_k are either all positive or all negative. The ground state of the model is then given by either the vacuum state ($\lambda > 1$) or by the state where all modes are occupied ($\lambda < 1$). In the intermediate regime, where some of the λ_k are positive and some of them are negative, the Hamiltonian has positive as well as negative eigenvalues. The ground state is then given by the state where all modes with negative λ_k are occupied and all the others are empty.

This behavior results in the effect that for $|\lambda| > 1$ the energy difference ΔE between the ground state and the lowest excited eigenstate is finite even in the thermodynamic limit $N \to \infty$. For such *gapped* systems it can be proven, using Lieb-Robinson bounds, that correlations in the ground state decay exponentially with the distance [28].

In the regime $|\lambda| \leq 1$, on the other hand, ΔE vanishes in the thermodynamic limit, which results in a critical phase with long-range interactions.

Covariance matrix of eigenstates and Gibbs state   By lemma 2 the covariance matrix of the Gibbs state in normal-form is given by

$$\gamma_{\text{Gibbs}}^{\text{n.f.}} = \bigoplus_{j=1}^{N} \tanh\left(\frac{1}{2}\beta\epsilon_j\right) J_2.$$

As seen in the discussion of the previous model, the covariance matrix of an eigenstate $|E_k\rangle = |k_1, \ldots, k_N\rangle$, if H is given in normal-form, is simply

$$\gamma_k^{\text{n.f.}} = \bigoplus_{j=1}^{N} (-1)^{k_j} J_2.$$

To get the representation of the two matrices in the original Majorana-operators we just need to transform like in eq. 27. This yields

$$\gamma_{\text{Gibbs}} = \frac{1}{i} \bar{W} S \left(U \oplus U\right) S^\top \gamma_{\text{Gibbs}}^{\text{n.f.}} S \left(U^\top \oplus U^\top\right) S^\top W^\dagger \tag{28}$$

and analogously for γ_k. So all that is necessary to calculate is the normal form of the coupling matrix $h^{\text{n.f.}}$ and the unitary transformation U. All the rest follows directly from eq. 28 and lemma 2.

5.1 Numerical experiments regarding ETH

To investigate whether the ETH holds for the XX-model I have conducted different numerical experiments, each in the critical regime with $\lambda = 0.25$. I only studied the subsystem composed of the first two spins/sites in the chain. Note that if the ETH does not hold for

subsystems of size 2 it cannot hold for subsystems that are bigger. Furthermore it does not matter which two neighboring spins are considered, because the system is translationally invariant.

Experiment 1 (Local inverse temperature vs. global energy) The first experiment studied whether the local inverse temperature depends smoothly on the energy of the total system. As discussed in section 2.2.1 this is necessary if the ETH can be considered as a plausible explanation of thermalization. The experiment was done in the following way. First a random eigenstate of the total system was chosen from the uniform distribution. Then the energy of total system E as well as the energy of the subsystem E_S was calculated using lemma 1. Then the covariance matrix $\gamma^\mathsf{S}_\mathrm{Gibbs}$ of the Gibbs state of the subsystem was calculated using only the upper left 4×4 sub-matrix h_S of h and β was chosen such that

$$\left| \frac{1}{2}\mathsf{Tr}\left(h_\mathsf{S}^\top \gamma^\mathsf{S}_\mathrm{Gibbs}\right) - E_\mathsf{S} \right| \leq 10^{-8}.$$

Finally the resulting inverse temperature β was plotted exemplary over the energy E of the total system in figure 1 (a-c) for $n = 10, 40, 90$. To analyse the results quantitatively I furthermore computed the principal components of the inverse temperature in dependence of the total energy. Then the standard-deviations σ_max and σ_min in direction of the maximal and minimal variance, respectively, was calculated and the ratio $r = \frac{\sigma_\mathrm{min}}{\sigma_\mathrm{max}}$ was plotted in figure 1 (d) for system sizes between $n = 10$ and $n = 90$. The ratio r can be viewed as a measure for the ratio of the short and long axis of the ellipse enclosing the cloud of datapoints. It is therefore a measure of how well the inverse temperature can be approximated by a smooth function of the total energy.

Experiment 2 (Local inverse temperature vs. local energy) As a sanity check for the computations in experiment 1 I also calculated the inverse temperature of the subsystem in dependence of the energy of the *subsystem*. Figure 1(e) shows an example-plot for a system size of $n = 10$. The results for larger systems are similar.

Experiment 3 (Eigenstate vs. local Gibbs state I) The second experiment directly checked the ETH. First a random eigenstate was chosen from the uniform distribution and the corresponding covariance matrix was calculated. Then the covariance matrix of the corresponding local Gibbs state was calculated in the same way as in experiment 1. After that, $\Delta\gamma_{1,2}$ and $\Delta\gamma_{1,4}$, the absolute values of the differences of the entries (1,2) and (1,4) of both covariance matrices, were calculated. Finally the results were sampled over 50 eigenstates and the mean of $\Delta\gamma_{1,2}$ and $\Delta\gamma_{1,4}$ were plotted over subsystem sizes $n = 5, \ldots, 40$ in figure 2(a). Note that $\gamma_{1,2}$ is the expectation value of the local magnetization, i.e. $\gamma_{1,2} = \langle Z_1 \rangle$.

Experiment 4 (Eigenstate vs. local Gibbs state II) This experiment was almost a repetition of experiment 3. Instead of choosing the eigenstates from the complete uniform distribution the eigenstates were restricted to those that have energy sufficiently far away from the mean. The reason is the following: When choosing eigenstates randomly from the uniform distribution, the probability to chose a state with energy close to the mean energy grows exponentially with the number of sites (cf. figure 1(a-c)). It is therefore necessary to artificially choose states with energies sufficiently far away from the mean to get more representative data. To do this, first 500 eigenstates were chosen from the uniform distribution for every n and the mean $\langle E \rangle$ and the standard-deviation σ of their energy was calculated. Then the experiment was restricted to be performed with eigenstates that have energies outside the interval $[\langle E \rangle - \sigma, \langle E \rangle + \sigma]$. The results are plotted in figure 2(b).
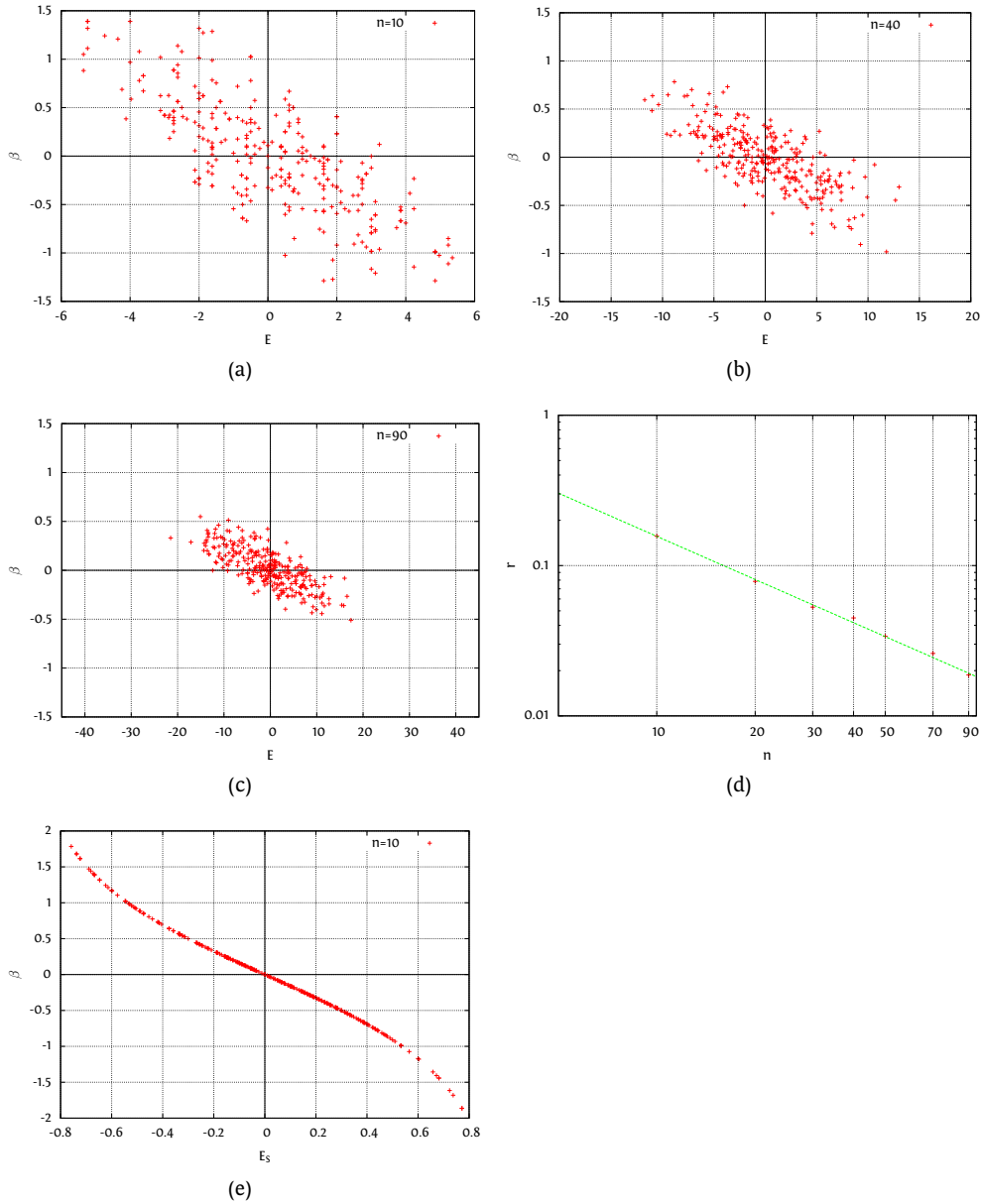
Figure 1: (a-c) Experiment 1. The plots show the local inverse temperature β of the first two spins in dependence of the energy of the total system E for system sizes $n = 10, 40, 90$.
(d) Ratio $r = \frac{\sigma_{\min}}{\sigma_{\max}}$ of the standard-deviation in direction of maximal and minimal variance of the principal components of the inverse temperature in dependence of the total energy. The quantities $\sigma_{\min}$ and $\sigma_{\max}$ are a measure for the length of the short and long axis, respectively, of an ellipse enclosing the clouds of datapoints (cf. (a-c)). The green line is given by a fit to a power-law with exponent ≈ -1.
(e) Experiment 2. The plot shows the local inverse temperature β of the first two spins in dependence of the energy of the *subsystem* E_S for system size $n = 10$.

Experiment 5 (Eigenstate vs. global Gibbs state) The last experiment studied a different notion of thermalization and is also closely connected to the role of conserved quantities.
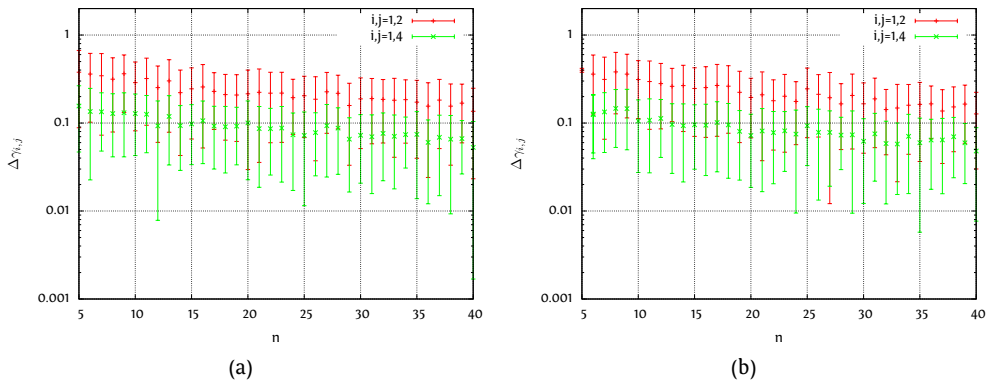
Figure 2: (a) Experiment 3. Mean of $\Delta\gamma_{1,2}$ and $\Delta\gamma_{1,4}$ (for def. see text) for the covariance matrices of an eigenstate and the local Gibbs state that has the same energy on the first two spins. Each data point is a sample over 50 randomly chosen eigenstates. The eigenstates were chosen from the uniform distribution. The error-bars are given by the standard deviation.
(b) Repetition of (a), but restricted to eigenstates with energies outside the interval $[\langle E \rangle - \sigma, \langle E \rangle + \sigma]$ (see text).

We know that if a subsystem of a large system equilibrates, its equilibrium state is given by the reduction of the maximum entropy state of the total system, under the constraint that the initial expectation values of *all* conserved quantities remain fixed. It is imaginable, however, that effectively only a small number of conserved quantities are important. Particularly it might be the case that only the total energy is of importance. Then the local system's state would be given by the reduction of the Gibbs state of the *total* system. To check if this is the case in the XX-model a very similar procedure as in the previous experiments was used. The difference lies in the fact that the reduction of the randomly chosen eigenstates was compared with the reduction of the global Gibbs state instead of the local Gibbs state. Furthermore, instead of comparing $\gamma_{1,2}$ and $\gamma_{1,4}$ separately, $||\Delta\gamma||_2$, the 2-norm of the difference of the local covariance matrices, was calculated. This was done for system sizes $n = 20, 30, 40, 55, 70, 85$. To be able to compare the results, $||\Delta\gamma||_2$ was also computed for two randomly chosen eigenstates. In both cases 100 samples were used for every n. The results are plotted in figure 3.

5.2 Discussion of the results

I will now discuss the results of the numerical experiments, beginning with experiment 1. The results of this experiment are plotted in figure 1(a-c). First note that due to the fact that the spectrum of the system is centered around 0 it is possible to get positive as well as negative energies on the subsystem. From figure 1 it is clear that the local inverse temperature of the subsystem does not vary smoothly with the energy of the total system for the system sizes considered. In fact, even for eigenstates of the total system with (almost) the same energy, the temperature can be very different on the subsystem.

   Comparing the plots for the three different system sizes $n = 10, 40, 90$ shows, however, that the scattering gets smaller with bigger system size. This indicates that the dependence of the local inverse temperature on the global energy might converge to a smooth curve for very large n. This can be seen even more clearly in figure 1(d), which indicates that the ratio $r = \frac{\sigma_{\min}}{\sigma_{\max}}$ converges in a power-law fashion to 0 for large n. Such a smooth variation of local inverse temperature with the total energy is necessary if the ETH should be considered as a plausible explanation for thermalization as discussed in section 2.2.1. Figures 1 (a-
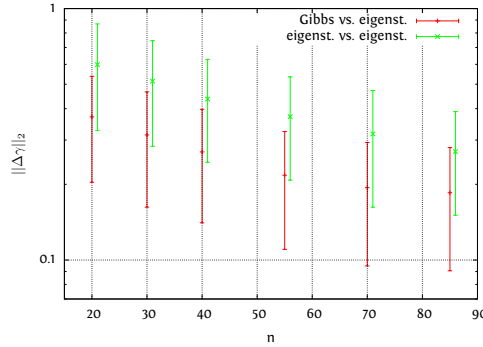
Figure 3: Experiment 5. Mean of $||\Delta\gamma||_2$ (for def. see text) for the local covariance matrices, on the first two spins, of an eigenstate and the corresponding *global* Gibbs state (red) or a second, randomly chosen, eigenstate (green). Each data point is a sample over 100 randomly chosen eigenstates. The eigenstates were chosen from the uniform distribution. The green datapoints were all moved one unit to the right for visual clarity. The error-bars are given by the standard deviation.

c) furthermore illustrate quite clearly the effect that randomly chosen eigenstates have energy close to the mean with a probability that grows exponentially with the system size.

Also note that the inverse temperature indeed varies smoothly with the *local* energy (see figure 1(e)) already for a small system of size $n = 10$. This should, of course, be the case because $\exp\left(-\beta H\right)$ is a smooth function of the inverse temperature.

Figures 2(a) and 2(b) show that the difference of the expectation value of the local magnetization (matrix-entry $\gamma_{1,2}$) computed from an eigenstate and the corresponding Gibbs state decreases exponentially with the system size. It is therefore plausible to say that the local magnetization thermalizes for single eigenstates. The same is true for the matrix-entry $\gamma_{1,4}$. The agreement of figures 2(a) and 2(b) furthermore indicates that the results not only hold for eigenstates with energies very close to the mean.

The last experiment (see figure 3) shows that an eigenstate of the Hamiltonian of the total system locally looks increasingly similar to the reduction of the global Gibbs state with same energy when the total system gets larger. In fact, this convergence is also roughly exponential in the system size. However, the same is true if one compares two randomly chosen eigenstates, although the absolute value of $||\Delta\gamma||_2$ is on average higher in this case. One has to be careful in interpreting this result, however, because choosing two eigenstates randomly yields two eigenstates with energy close to the mean energy with a probability that grows exponentially with the system size. If the ETH is true, which the previous results indicate, then these eigenstates locally look like Gibbs states with similar temperature and should therefore be locally very similar. A similar effect would occur when the eigenstates were restricted to energies outside a certain interval that encloses the mean energy. The only difference would lie in the fact that the randomly chosen eigenstates would cluster at the edge of that interval. It is therefore not clear if the local similarity of an eigenstate and the corresponding Gibbs state is just a result of this concentration of measure effect.

Concluding, the experiments indicate that, in the XX-model, thermalization indeed already occurs on the basis of eigenstates if the total system is very large.

6 Conclusions

In this thesis I studied the problem of equilibration, thermalization and the role of conserved quantities in two models.

The first model was an interaction-free spin chain with local magnetic fields. By conjugating it with a unitary operator, interactions between neighboring spins were introduced. This model can be expected to thermalize from general arguments. I showed analytically that the equilibrium expectation values of local observables on any subsystem S can be computed by using the state that maximizes entropy subject to the constraint that the expectation values of all *local* conserved quantities on S and its boundary agree with the initial conditions. The main technical reason for this was, that the interaction was given by tensor products of traceless Pauli operators. This result shows that the equilibrium state of a small subsystem does not always depend on subsystems that are far away.

Furthermore by transforming the model into one of free fermions and using the property that eigenstates of free fermionic systems are Gaussian, it was possible to show analytically that the Eigenstate Thermalization Hypothesis cannot hold for subsystems of size ≥ 2.

The second model was the fermionic XX-model in the critical regime, with $\lambda = 0.25$. In this case, numerical experiments were used instead of analytical methods. The fact that the model is a free fermionic model made it possible to work with covariance matrices instead of exact diagonalization techniques. This way numerical experiments for systems up to system-sizes of 90 sites could be done. The results of the experiments indicate that thermalization can indeed be viewed as already happening at the level of eigenstates if the total system is very large. They therefore support the ETH. This is particularly interesting as the result is a counter-example for the paradigm that integrable systems do not thermalize and especially do not thermalize according to the ETH.

A natural question for further research is to ask whether it is possible to find general arguments that explain when the ETH holds. One possible guide in this direction could be to ask how well a state is actually defined if the expectation values of all local observables are given. Furthermore it would be interesting to ask if it is possible to find general criteria that determine if all conserved quantities have to be considered in the process of equilibration and thermalization for a given system.

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Erklärung

Hiermit versichere ich, dass ich die vorliegende Arbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe, und dass alle Stellen der Arbeit, die wörtlich oder sinngemäß aus anderen Quellen übernommen wurden, als solche kenntlich gemacht sind.

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