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Summary

A numerical study of a system of spinless fermions on a two dimensional lattice is performed. The system is small enough such that exact diagonalization up to machine precision can be applied. The aim is to study the equilibration and thermalization of closed quantum systems by looking at the expectation values of certain observables, a topic which lies at the foundations of statistical mechanics but has recently become also of great experimental interest. In particular the eigenstate thermalization hypothesis (ETH) is being tested, a proposal that thermalization of quantum systems takes place at the level of individual energy eigenstates and which has been conjectured for Hamiltonians far from integrability. By changing the interactions between the particles the system is moved away from the integrable free fermion model and the validity of the ETH is being inferred. In addition indicators of quantum chaos are being studied. These measure how far a system is from integrability and have been proposed to be tightly linked to eigenstate thermalization. In particular we are looking at level spacing statistics and delocalization measures of energy eigenstates with respect to the eigenbasis of the free fermion system.
Before presenting the results of our computations the required theoretical concepts are introduced.

Zusammenfassung

Eine Studie eines Systems spinloser Fermionen auf einem zweidimensionalen Gitter wird gemacht. Da das zu untersuchende system klein genug ist kann eine exakte Diagonalisierung bis zur Maschinenpräzision durchgeführt werden. Das eigentliche Ziel ist es die Thermalisierung abgeschlossener Quantensysteme zu untersuchen indem man die Erwartungswerte gewisser Observablen betrachtet. Dieser Themenkreis ggehört zu den Grundlagen der statistischen Physik, wurde aber in den letzten Jahren immer mehr auch von experimentellem Interesse. Konkret wird hauptsächlich die eigenstate thermalization hypothesis ETH getestet. Diese besagt dass sich Thermalisierung von Quantensystemen auf der Ebene der Eigenzustände vollzieht und wurde vorhergesagt für Systeme die weit entfernt sind von Integrabilität. Indem man die Stärke der Wechselwirkung zwischen den Telchen variiert bewegt man das System weg von der Integrabilität freier Fermionen und die Gültigkeit der ETH kann getestet werden. Zusätzlich werden Indikatoren von quantenchaotischem Verhalten untersucht. Diese messen wie weit weg von Integrabilität sich ein System befindet und wurden mit der ETH in Verbindung gebracht. Dabei geht es konkret um die level spacing statistcs und um Maße für die Delokalisireung von Energieeigenzuständen in Bezug auf die Eigenbasis des freien Systems.
Bevor die Ergebnisse präsentiert werden, werden die notwendigen theoretischen Konzepte eingeführt und erläutert.

1 Introduction

The ability to cool, trap and control the physical parameters of atomic gases has opened up new possibilities for many body physics [1]. The extremely low temperatures and low densities achieved mean that these gases can be considered as nearly perfectly isolated from the environment for considerable time scales. This has for the first time opened up the possibility to experimentally study closed macroscopic quantum systems out of equilibrium. Especially the long standing question of thermalization of these systems could be addressed in experiments for the first time in the history of physics ([2],[3]).

The question of thermalization has to do with the fact why large systems relax after some time to stationary states which can be described with one of the well known ensembles of quantum statistical mechanics. In contrast to classical statistical mechanics, where a satisfactory solution to this problem exists [4], no general solution has been found in the quantum case [56]. The main conceptual difficulty being the seemingly incompatibility with unitary time evolution.

Quite recently new concepts were proposed how the tackle this puzzle ([25],[31],[28], [47],[37]). One of the most studied of these new concepts is the eigenstate thermalization hypothesis (ETH), which states that thermalization in quantum mechanics happens at the level of individual energy eigenstates. The very influential work [5] proposed to test the ETH numerically using a system of particles on a lattice small enough such that exact diagonalization could be performed. Other studies followed and soon a new paradigm arose which states roughly that systems far away from integrability should thermalize through the eigenstate thermalization hypothesis whereas integrable models should not. It must be noted however that the notion of quantum integrability (in simple terms systems possessing many conserved quantities) is at first a much less clear cut concept than its classical counterpart and requires some clarification.

It is the aim of this work to test this paradigm numerically applying exact numerical diagonalization. For this a system of particles on a $2d$ lattice is considered, very similar to the one in [5]. In contrast to hardcore bosons however we are looking at systems of interacting spinless fermions. By varying the interaction strength we move the system away from the integrability of the free fermion model and observe how properties of the system change. One of the studies we will perform on our models is the time evolution of the expectation value of an observable following a quantum quench. This corresponds to first start the system in some eigenstate of the Hamiltonian. By changing some parameter in the Hamiltonian the system starts to evolve in time. This is especially interesting since quantum quenches are being applied in the above mentioned experiments on cold atomic gases.

To give a short overview, before presenting our results in section 3 we are going to introduce the required theoretical concepts used in our studies in section 2.

First we will define the concept of equilibration, the fact that in the long term a system can often be described by a stationary state. We will explain how this is compatible with the unitarity and time reversal invariance of quantum mechanics and state the main known general results about equilibration. These results will be tested in our numerical computations. Then we are going to explain in what sense this stationary state can be taken as a thermal state. This is where we are going to introduce the eigenstate thermalization hypothesis in its various variants. To provide some justification for the ETH we will discuss the recently revived notion of typicality, which states that thermal behaviour is in a sense a typical property of a quantum state (pure or mixed). Both concepts of equilibration and thermalization will be defined in for the expectation values of observables and the distinguishability of states with respect to measurements. Finally we will provide a proper definition of quantum integrability suited for our purposes. To measure how far a system departs from integrability quantities will be introduced that previously appeared in the study of quantum chaos, namely level spacing distributions and delocalization measures of energy eigenstates with respect to some basis. The change in these quantities has been conjectured to go hand hand with a change in the thermalization properties as one moves away from integrability [61]. One of the main aims of our studies is to test this conjecture and how accurately it applies to the systems described above.

2 Theoretical background

2.1 The problem of thermalization in quantum systems

For macroscopic quantum systems it is in general impossible to determine the exact form of the many body state and as well as the exact time evolution. However it is an experimentally well established fact that macroscopic quantum systems are well described (expectation values of observables, correlation functions,..) in their long time behaviour by the predictions of quantum statistical mechanics. The 'textbook' way of dealing with this problem is, instead of looking at the 'real' microstate of the system, represented by a vector in Hilbert-space, to introduce a statistical ensemble (the macrostate) [7]. This corresponds to a formal copies of the same system described by a density operator ρ_{Ensemble}, in analogy with the classical phase space density $\rho_{cl}(p, q, t)$ in classical phase space. All system properties are then to be averaged over the individual copies. The ensemble evolves in time according to the Von Neumann-equation

$$i\hbar \frac{\partial}{\partial t} \rho_{\text{Ensemble}} = -[\rho_{\text{Ensemble}}, H] \tag{2.1.1}$$

where H is the system Hamiltonian. The time independent equilibrium solution ρ_{eq} is then assumed by plausibility to be the microcanonical ensemble, where every energy eigenstate from a narrow energy shell is equally probable.

However, level populations are constants of motion. This means that they must have the same values for the, in general, far from equilibrium initial ensemble as well as for the equilibrium one. But this is very unlikely to be the case for the 'real' system and its 'real' time evolution. It is thus necessary to clarify the physical meaning of the thermal ensemble ρ_{eq} since it cannot be seen as a state the real system evolves into under the ordinary unitary time evolution. Thermalization must as such be given an operational definition which goes beyond unitary time evolution.

It is therefore the aim of these following chapters to try to define and explain the phenomena of equilibration and thermalization of closed systems (and their subsystems) by looking at the time evolution of the 'real' initial states according to the general rules of quantum mechanics. Since the details of the 'real' system are unknown, but statistical mechanics has proven to apply to many systems, it is to be expected that general features of these system are sufficient to describe these phenomena.

2.2 Basic set up

In this chapter we will now first lay down the general features of quantum systems that are necessary for the definition and study of the concepts of equilibration and thermalization in the sense described above.

2.2.1 Systems and Hamiltonians

The systems we are mainly interested in are condensed matter systems and systems of cold atoms on optical lattices. These can be described by spins or systems of particles (fermions, bosons) on a lattice. Since we are mainly interested in closed systems, we will consider systems with a finite number of degrees of freedom f and a finite dimensional Hilbert space $\mathcal{H}$. Most such systems in nature have short ranged interactions. The general Hamiltonian of such systems can be written as

$$H := \sum_{n=0}^{d-1} E_n |n\rangle\langle n| \tag{2.2.1}$$

where d is the dimension of $\mathcal{H}$ and the eigenvalues E_n are assumed to be ordered

$$E_0 \leq E_1 \leq E_2 \leq ... \tag{2.2.2}$$

with E_0 the ground state energy. In the case of *degenerate energies*, we write the projector P_E to the degenerate eigenspace with energy E as

$$P_E := \sum_{E_m = E} |m\rangle\langle m| \tag{2.2.3}$$

where the sum is over all eigenvalues satisfying $E_m = E$. The Hamiltonian can then be written as

$$H = \sum_{E_n} E_n P_{E_n} \tag{2.2.4}$$

where the sum is only over mutually different E_n-values, such that degenerate energies only appear once. We will call d' the number of different energy values.

A property which turns out to be very important for equilibration and which is believed to be of a generic character is the so called *non-degenerate energy gaps* condition (also called *non-resonance* condition). It says that for every $k, l, m, n \in (0, d-1)$

$$E_k - E_l = E_m - E_n \Longrightarrow (k = l \text{ and } m = n) \text{ or } (k = m \text{ and } l = n), \tag{2.2.5}$$

meaning that every energy gap $E_m - E_n$ appears exactly once in the spectrum of H. Keep in mind that the condition still admits degenerate energies, for example in systems with symmetries. The following intuitive argument is given for why it is believed that this property is generic [7]: if one takes a path $H(\lambda)$ in the 'space of all Hamiltonians', parametrized by λ, then every energy gap $E_m - E_n$ evolves differently to all other energy gaps as a function of λ. While crossings cannot be excluded in general, these special points will be of measure zero. This means that Hamiltonians with degenerate energy gaps will be of measure zero compared to all Hamiltonians.

Systems possessing a large number of degenerate energy gaps are integrable models [53], consisting of interacting subsystems, for example non-interacting particles on a lattice. Excluding such non-interacting particles was one of the main motivations for the non-degenerate energy gaps condition, since small subsystems of these systems cannot equilibrate.

2.2.2 Initial states and time evolution

In quantum mechanics the general state of a system is described by a density operator ρ. This includes mixed and pure states as special cases. With the unitary propagator

$$U_t := \exp(-iHt/\hbar) = \sum_{n=0}^{d-1} \exp(-iE_n t/\hbar)|n\rangle\langle n| \tag{2.2.6}$$

the time evolution of such a state can be written as

$$\rho(t) := U_t \rho(0) U_t^\dagger \tag{2.2.7}$$

where $\rho(0)$ is any initial state. Denoting the matrix elements of $\rho(t)$ by

$$\rho_{mn}(t) := \langle m|\rho(t)|n\rangle \tag{2.2.8}$$

yields

$$\rho(t) = \sum_{m,n=0}^{d-1} \rho_{mn}(0)|m\rangle\langle n| \exp(-i[E_m - E_n]t/\hbar) \tag{2.2.9}$$

The mean (ensemble averaged) level populations p_n of the energy eigenstates $|n\rangle$, which are constants of motion, can then be written as

$$p_n := Tr\{|n\rangle\langle n|\rho(t)\} = \rho_{nn}(t) = \rho_{nn}(0) \tag{2.2.10}$$

In a similar way, the mean occupation p_{E_n} of the energy E is given by

$$p_E := Tr\{P_E \rho(t)\} = \sum_{E_m = E} \rho_{mm}(t) = \sum_{E_m = E} p_m \tag{2.2.11}$$

The state $\rho(t)$ fulfils the normalization condition

$$1 = Tr\{\rho(t)\} = \sum_{n=0}^{d-1} \rho_{nn}(t) = \sum_{n=0}^{d-1} p_n = \sum_{E_n} p_{E_n} \tag{2.2.12}$$

One very useful property can be obtained by considering the fact that $P_{E_n}\rho(0)P_{E_n}$ commutes with H. This means that there is a basis of the subspace of energy E_n, where both operators are diagonal. Doing this for all the energy subspaces leads to a new complete basis of energy eigenstates, which can labelled as $|E_n, r_j\rangle$, where r_j is the degeneracy index. The normalization of this new set can then be written as $\langle E_n, r_j|E_m, r_k\rangle = \delta_{E_n E_m}\delta_{r_j r_k}$. For the matrix elements of ρ we get

$$\rho_{E_n, r_j E_m, r_k} = 0 \text{ if } (r_j \neq r_k \wedge E_m = E_n) \tag{2.2.13}$$

2.2.3 Subsystems

For us subsystems will usually be systems corresponding to subsets of the set of lattice points of the whole lattice. For any state ρ states of such subsystems correspond to the *reduced states*, which are defined [11] as the unique quantum states ρ^S with the property that for every observable A^S of the subsystem

$$\mathrm{Tr}_S(A^S\rho^S) = \mathrm{Tr}\{A^S\rho\}, \tag{2.2.14}$$

where Tr_S is the trace over the states of the subsystem. In the case of spinsystems the Hilbert space of the whole system is the tensor product of the Hilbert space of the subsystem and its complement (bath). The state reduction then corresponds to the partial trace,

$$\rho^S = \mathrm{Tr}_B\{\rho\}, \tag{2.2.15}$$

where Tr_B is the trace over the states of the bath. For fermions and bosons the Hilbert space of the whole system is not the tensor product of the subsystem and bath. This is so because of the indistinguishability of the particles. The Hamiltonian H of whole system can then be written as

$$H = H_0 + H_I = H_S + H_B + H_I \tag{2.2.16}$$

where H_S (H_B) is the Hamiltonian of the system (bath) and H_I is the Hamiltonian which describes the interaction between system and bath.

It is important to stress that the time evolution of the state of the subsystem is in general not unitary any more.

2.2.4 Experimental conditions

The important question is now how realistic initial states look like for experiments with closed quantum systems. This knowledge can then be used to estimate equilibration time scales (see section 2.3.4). For that, one has to consider the fact that even for closed systems the *preparation* of the initial condition happens through interaction with the environment ([7], [8], [9]). This leads to entanglement between the system and environment, which means that the system will start in a mixed state even for a single realization of the experiment. Closing the connection to the outside then usually leads to a diffusive spreading of the occupations over neighbouring energy levels [7]. For macroscopic systems the number of degrees of freedom $f \approx N_A$, where $N_A := 6 \times 10^{23}$ is *Avogadro's number*. The average energy spacing between neighbouring energy levels scales typically approximately like $10^{-\mathcal{O}(f)}$ [18]. This is a huge number of energy levels (of the order of $10^{\mathcal{O}(f)}$) on any energy scale one encounters in today's physics, usually a few joules in closed system experiments. Even if it were possible to prepare a state with an energy width as small as for example $10^{-10^{22}}$J, there would still be roughly $10^{0.9\times 10^{23}}$ states within that interval.

It is then plausible to assume [7], that the above mentioned diffusive spreading of level populations will randomize the p_n's in such a way that they can be written as

$$p_n = h(E_n) + \delta p_n, \tag{2.2.17}$$

where $h(E)$ is a smooth function which corresponds to an averaging of the p_n's over local energy intervals. It is independent of the exact choice of the intervals, which are small compared to the experimental (global) energy scale, but still entail a huge number of energy states. The δp_n are 'unbiased fluctuations' such that their average over an interval is very small compared to $h(E)$ of that interval.

One can estimate (in a heuristic way) from 2.2.17 the typical maximum value of the p_n's in an experimentally realistic initial state [7]. The easiest way is to first assume that one has exactly $10^{\mathcal{O}(f)}$ states per Joule and that $h(E)$ is approximately constant over the whole energy range. We can then deduce from the normalization condition 2.2.12 that $h(E)$'s value must be $10^{-\mathcal{O}(f)}$. Since $h(E)$ is the local average of the p_n, the individual p_n can hardly get much bigger than about $10^{10^{22}} h(E)$. Otherwise the local average of the δp_n could not be small compared to $h(E)$ for any choice of the intervals. From this we deduce that

$$\max_n \; p_n = 10^{-\mathcal{O}(f)}. \tag{2.2.18}$$

In general, $h(E)$ can vary fast on the global experimental scale and the occupations differ strongly. It is however reasonable to assume that they still remain small and that 2.2.18 still holds.

Because for most realistic Hamiltonians the degeneracies of the spectrum are much smaller than $10^{\mathcal{O}(f)}$, we can deduce from 2.2.18 that typically

$$\max_{E_n} \; p_{E_n} = 10^{-\mathcal{O}(f)}. \tag{2.2.19}$$

This statement is independent of the chosen energy basis. These maximum populations will turn out to be crucial for equilibration time scales.

Exceptions to such small maximum populations can arise at very low temperatures where the ground state probability might be significantly larger [10]. In such cases, one has

$$\max_{E_n}{}' \; p_{E_n} = 10^{-\mathcal{O}(f)}, \tag{2.2.20}$$

where the prime indicates that the largest p_n is not included in the maximization. Other exceptional situations are systems with energy gaps or levels with very high degeneracies.

All this shows that it is nowadays experimentally impossible to prepare states of closed macroscopic systems which have an overlap with only a small number of energy eigenstates. Another argument in this direction comes from the

time-energy uncertainty [19].

$$\Delta E \sim \frac{\hbar}{\Delta t}. \tag{2.2.21}$$

To prepare a single eigenstate, ΔE would have to be of the order of the spacing between two neighbouring energy values, which is about $10^{-\mathcal{O}(f)}$. That means that an astronomically long time would be needed to prepare such a state. And even if one was to perform an ideal energy measurement, leading to an exact eigenstate, one has to keep in mind the finite measurement resolution. This again leads to a significant population of many levels.

2.2.5 Observables and measurements

General observables are Hermitian operators and are written in the usual way as

$$A := \sum_{m,n=0}^{d-1} A_{mn}|m\rangle\langle n| \tag{2.2.22}$$

where

$$A_{mn} := \langle m|A|n\rangle. \tag{2.2.23}$$

Expectation values in an arbitrary state $\rho(t)$ are given by

$$\langle A\rangle_{\rho(t)} := Tr\{\rho(t)A\} \tag{2.2.24}$$

Realistic measurement devices have a *finite range* of possible measurement outcomes (even in the case of infinite dimensions) which can be defined as [7]

$$\Delta_A := \max_{\Psi\in S(\mathcal{H})} \langle\Psi|A|\Psi\rangle - \min_{\Psi\in S(\mathcal{H})} \langle\Psi|A|\Psi\rangle = a_{\max} - a_{\min} \tag{2.2.25}$$

where $S(\mathcal{H})$ is the set of normalized vectors in $\mathcal{H}$ and $a_{\max}$ and $a_{\min}$ are the maximal and minimal eigenvalues of A.

Additionally a measurement device has a *finite resolution* δA. Every measurement known to date yields less than 20 relevant digits [7], i.e.

$$\frac{\Delta_A}{\delta A} \leq 10^{20} \tag{2.2.26}$$

Observables represented by Hermitian operators are not the most general form of a measurement possible in quantum mechanics. These are the so called *positive operator valued measures* (POVM) [20]. A general measurement M is described by giving a positive operator M_a to every measurement outcome a with the normalization condition

$$\sum_a M_a = Id. \tag{2.2.27}$$

The probability of obtaining outcome a in a state ρ is given by

$$p_a := Tr\{\rho M_a\}. \tag{2.2.28}$$

In the case of observables A, the M_a correspond to the projectors of the corresponding eigenspaces of A. For this reason these types of measurements are called *projective measurements*. All this can be generalized to continuous measurement outcomes. In realistic situations these can be modelled by discrete ones with the number of possible outcomes given by $\frac{\Delta_A}{\delta A}$.

2.2.6 Thermal states

In this section, we will define and describe the statistical ensembles known from statistical mechanics. We will also sketch the usual derivation of the canonical ensemble for the state of a subsystem if the whole system is in the microcanonical state and point out the problems associated with it. This is done as preparation for later chapters where we will speak of thermalization when the system is in some sense close to one of these thermal states.

Microcanonical ensemble:

It is defined with respect to a Hamiltonian $H = \sum_{E_k} E_k P_{E_k}$ and an energy interval $I_{E,\Delta} := [E - \Delta/2, E + \Delta/2]$. The corresponding density matrix is given by

$$\rho_{\mathrm{mc}}[H](E,\Delta) := \frac{\sum_{k:E_k \in I_{E,\Delta}} P_k}{Z_{\mathrm{mc}}[H](E,\Delta)}. \tag{2.2.29}$$

Here $Z_{\mathrm{mc}}[H](E,\Delta)$ is the microcanonical partition function given by

$$Z_{\mathrm{mc}}[H](E,\Delta) := \mathrm{Tr}\{\sum_{k:E_k \in I_{E,\Delta}} P_k\} = \dim(\mathcal{H}_{E,\Delta}), \tag{2.2.30}$$

where $(\mathcal{H}_{E,\Delta})$ is the space spanned by the energy eigenstates with energies in $I_{E,\Delta}$. The *von Neumann entropy* of a quantum state ρ is defined as

$$S := -k_B \mathrm{Tr}\{\rho \log \rho\}, \tag{2.2.31}$$

where k_B is the *Boltzmann constant*. For the microcanonical state one has

$$S = k_B \log Z_{\mathrm{mc}}[H](E,\Delta). \tag{2.2.32}$$

It is the unique state which maximizes S under restriction of the energy range. The temperature is given by

$$\frac{1}{T} := \frac{\partial S}{\partial E}. \tag{2.2.33}$$

Canonical ensemble:

The canonical density matrix (also called Gibbs state) is defined as

$$\rho_G[H](\beta) := \frac{\exp(-\beta H)}{Z_G[H](\beta)}, \tag{2.2.34}$$

where $\beta \in \mathbb{R}$ and $Z_G[H](\beta)$ is the canonical partition function given by

$$Z_G[H](\beta) := \mathrm{Tr}\{\exp(-\beta H)\}. \tag{2.2.35}$$

The Gibbs state is the unique maximum entropy state given a fixed mean energy E_{mean}. The corresponding β is a Lagrange multiplier determined by the condition

$$E_{\mathrm{mean}} := \langle \Psi(0)|H|\Psi(0)\rangle = \mathrm{Tr}\{\rho_G[H](\beta)H\}. \tag{2.2.36}$$

For a finite system the two ensembles give in general different results. This has to do with the fluctuations of the energy in the canonical ensemble. However in the thermodynamic limit, where the number of particles (spins) $N \to \infty$, while the density N/V is kept constant, the canonical probability is so sharply peaked around the mean energy that the ensemble becomes essentially indistinguishable from the microcanonical one. This can be seen as follows [24].

From the definition of canonical density matrix $\rho_G[H](\beta)$ one obtains for the mean energy in the Gibbs state

$$E_{\mathrm{mean}} := \langle H \rangle_{\rho_G} = -\frac{\partial \log \rho_G[H](\beta)}{\partial \beta}. \tag{2.2.37}$$

Similarly one gets for the mean squared deviation of the energy

$$E^2_{\mathrm{var}} := \langle H^2 \rangle_{\rho_G} - \langle H \rangle^2_{\rho_G} = \frac{\partial^2 \log \rho_G[H](\beta)}{\partial \beta^2} = -\frac{\partial \langle H \rangle_{\rho_G}}{\partial \beta} = k_B T^2 C_X, \tag{2.2.38}$$

where

$$C_X := \frac{\partial \langle H \rangle_{\rho_G}}{\partial T} \tag{2.2.39}$$

is the specific heat and X stands for the set of generalized displacements (volume, magnetic field,...). Since C_X is an extensive quantity (it is the quotient of the extensive energy and the intensive temperature), we have that $E_{\mathrm{var}} \propto N^{1/2}$. It follows that the relative error

$$\frac{E_{\mathrm{var}}}{E_{\mathrm{mean}}} \propto N^{-1/2}. \tag{2.2.40}$$

This means that for large N the canonical probability distribution (as a function of energy) is sufficiently sharp around the most probable energy which can then be identified with the mean energy E_{mean}. Thermodynamic potentials then usually differ from their microcanonical values by terms proportional to $\log N$. These terms than become less significant as $N \to \infty$, such that the two ensembles become more and more identical.

We are now going to review the derivation of the Gibbs ensemble [11] and point out some crucial difficulties that one encounters when dealing with large

quantum systems. We will do so only for the case of spin systems (the derivation for indistinguishable particles using properties of creation and annihilation operators can be found in [11]).

As already explained above, the main assumption is that the whole system (system + bath) is in a microcanonical state on some narrow energy interval $I_{E,\Delta}$. Narrow means that the interval is small compared to the experimental energy scale but still contains many energy eigenstates.

Another important assumption is the weakness of the interaction between system and bath. One could argue for eigenstates of H_0 to be good approximations for eigenstates of the total system. This is however a very problematic assumption for the following reason.

The eigenstates of H_0 can be taken as products of eigenstates of the system and the bath (because of the tensor product nature of the Hilbert space for spins). In general, when the interaction H_I is weak compared to the measurement resolution (or energy uncertainty) one can expect the shift of the eigenenergies of H compared to those of H_0 to be small. In the case of short range interactions, the strength of H_I will scale like the boundary between system and bath, while H_0 will scale like the volume. By increasing the total system size, one can thus make the interaction small. However, even when the interaction is weak, the form of the eigenstates will change strongly compared to those of H_0. This has again to do with the fact that the gaps between the eigenstates is exponentially small in the number of degrees of freedom f. This means that conventional perturbation theory will usually break down, because even if the interaction is small in the above sense there will still be of the order of 10^f eigenstates of H_0 in that energy window. The eigenstates of H will then in general be superpositions of all these eigenstates.

Putting these difficulties aside for now and ignoring the interaction term, the spectral projectors of H_0 have the form

$$P_{E_k^0} = \sum_{l,m:E_l^S+E_m^B=E_k^0} |E_l^S\rangle\langle E_l^S| \otimes |E_m^B\rangle\langle E_m^B|, \tag{2.2.41}$$

where $|E_l^S\rangle$ and $|E_m^B\rangle$ are eigenstates of the system and the bath respectively. For the microcanonical state we then get (ignoring the normalization)

$$\rho_{mc}[H_0](E,\Delta) \propto \sum_{k:E_k^0\in I_{E,\Delta}} \sum_{l,m:E_l^S+E_m^B=E_k^0} |E_l^S\rangle\langle E_l^S| \otimes |E_m^B\rangle\langle E_m^B|. \tag{2.2.42}$$

The reduced state of the system can now be computed as the partial trace with respect to the bath, $\rho^S = \mathrm{Tr}_B\{\rho_{mc}[H_0](E,\Delta)\}$. This gives the result

$$\rho^S \propto \sum_l \dim(\mathcal{H}_l^B)|E_l^S\rangle\langle E_l^S|, \tag{2.2.43}$$

where $\mathcal{H}_l^B := \mathcal{H}^B_{E-E_l^S,\Delta}$ is the spectral subspace of $\mathcal{H}^B$ associated with eigenenergies of H^B in $I_{E-E_l^S,\Delta}$. If now for some $\beta \in \mathbb{R}$

$$\dim(\mathcal{H}^B_{E,\Delta}) \propto \exp^{-\beta E}, \tag{2.2.44}$$

then

$$\rho^S \propto \rho_G[H_S](\beta). \tag{2.2.45}$$

This means that β, which was introduced as a parameter measuring the number of states of the bath becomes the inverse temperature of the thermal state $\rho_G[H_S](\beta)$ of the subsystem.

The relation 2.2.44 is a general property of large quantum systems and can be derived as a consequence of the extensivity of the Von Neumann entropy [56]. For the energy of a large system, extensivity is a consequence of the fact, as explained above, that the interaction H_I becomes very small compared to the total energy, at least for short range interactions. More generally it seems plausible to divide any large system into a very big number N of parts (subsystems), such that the individual parts are almost non interacting, even though the individual constituents (particles, spins) might interact strongly. (However one has to be cautious, because we have seen that the eigenstates of large systems can change dramatically even for weak interactions.) The density of states of the total system can then be approximately computed as the convolution of the state densities of the individual parts (the density of states can be basically seen as the limit of the number of states $\dim(\mathcal{H}_{E,\Delta})$ for small Δ and large particle number)

$$G(E) \approx \int \cdots \int g(E_1)g(E_2 - E_1) \dots g(E_i - E_{i-1}) \dots g(E - E_{N-1}) \prod_{i=1}^{N-1} dE_i, \tag{2.2.46}$$

where E_i are the total energies of the first i parts and g are the state densities of the individual parts. From this one can deduce an approximately Gaussian form for the state density as a function of energy and the extensivity of the entropy, which is essentially the logarithm of the density of states [56]. Formally, one writes

$$S(E, V) = Ns(E/N, V/N), \tag{2.2.47}$$

where S, E, V are the entropy, energy and volume of the total system and s is the entropy of the individual parts. Expanding now $S(E)$ around some fixed energy per particle $\epsilon := E_0/N$ [56]

$$k_B \log(\dim(\mathcal{H}_{E,\Delta})) = S(E) \approx Ns|_\epsilon + \frac{ds}{dE}\Big|_\epsilon (E - E_0) + \frac{1}{2N}\frac{d^2 s}{(dE)^2}\Big|_\epsilon (E - E_0)^2 + O(\epsilon^3). \tag{2.2.48}$$

Applying the chain rule of differentiation one obtains the crucial result that terms of order n in the expansion scale like N^{1-n}. Therefore it is justified to truncate after the linear term since N was assumed to be large. Defining now

$$\beta := \frac{1}{k_B}\frac{ds}{dE}\Big|_{\epsilon}, \tag{2.2.49}$$

the desired result 2.2.44 for the number of states is obtained. For a more rigorous derivation see [21].

Coming now back to the question about the validity of the above derivation in the case of an interaction H_I between system and bath. Recently an upper bound on the mistake that one makes when ignoring this interaction has been obtained [21]. More specifically it was found for the trace distance

$$\mathcal{D}(\rho^S, \rho_G[H_S](\beta)) \in O((\beta||H_I||_\infty)^{1/2}), \tag{2.2.50}$$

where $\rho^S := \mathrm{Tr}_B\{\rho_{mc}[H](E,\Delta)\}$. This means that $\mathcal{D}$ scales like the left hand side of eq. 2.2.50. The condition for the validity of the above statement is that the interaction is weak enough such that

$$||H_I||_\infty \ll \frac{1}{\beta} \ll \Delta. \tag{2.2.51}$$

However, the weakness of this statement is that while $||H_I||_\infty$ is an extensive quantity, $1/\beta$ is intensive. If we enlarge the whole system the interaction between S and B scales with their boundary but the temperature remains the same, meaning at some point the interaction becomes larger than $1/\beta$ and the statement does not apply. This contradicts our intuition that scaling the total system should not change the thermal state of the subsystem.

Generalized Gibbs ensemble:

If a system has the property that there is a set of algebraically independent operators $\{I_k, k = 1, ...n < d\}$ such that $[I_k, I_l] = 0\ \forall l, k$ and the Hamiltonian H is a member of that set, we define the *generalized Gibbs state* by

$$\rho_{GGE}[\{I_k\}](\{\beta_k\}) := \frac{\exp\left(-\sum_k \beta_k I_k\right)}{Z_{GGE}[\{I_k\}](\{\beta_k\})}, \tag{2.2.52}$$

where

$$Z_{GGE}[\{I_k\}](\{\beta_k\}) := \mathrm{Tr}\{\exp\left(-\sum_k \beta_k I_k\right)\} \tag{2.2.53}$$

is the generalized canonical partition function. The fact that the I_k's commute with H means that they are integrals of motion. In analogy to the Gibbs ensemble, the generalized Gibbs ensemble has the maximum entropy [52] among all

states with fixed values n_k of I_k. The β_k's are Lagrange multipliers determined by the conditions

$$n_k := \langle\Psi(0)|I_k|\Psi(0)\rangle = \mathrm{Tr}\{\rho_{GGE}[\{I_k\}](\{\beta_k\})I_k\} \tag{2.2.54}$$

for all k. For the relation of the generalized Gibbs ensemble to the concept of integrability see section 2.5.2.

2.3 Equilibration

2.3.1 Equilibration of expectation values

We will now define a concept of equilibration which is fully compatible with unitary quantum mechanical time evolution including the time reversal symmetry. In order to speak of equilibrium, $\rho(t)$ has to, in some sense, reach a time independent state ω. However if the system starts in some time dependent initial state ρ_0, no time independent state state can be approached in the long time limit. This is because of the so called *recurrence* property of the unitary time evolution [37], which is always present in finite dimensional systems (for pure and mixed initial states): there are always arbitrarily large t for which the state returns arbitrarily close to its initial value (*quasi-periodicity*). The same is true for expectation values of observables and for the reduced states of subsystems of the system.

We can say that in this sense equilibration and quantum mechanics are incompatible. One way out is to consider the following situation. The system spends most of the time close to the equilibrium state ω, in the sense that if there are larger excursions, these will be very short in time (compared to the total time interval), followed by long times spent close to equilibrium. In such a situation ω should be approximately equal to the infinite time-average of $\rho(t)$.

More formally, we define the time average for states

$$\begin{aligned} \langle\rho(t)\rangle_T &:= \frac{1}{T}\int_0^T \rho(t)dt \\ \langle\rho(t)\rangle_\infty &:= \lim_{T\to\infty}\langle\rho(t)\rangle_T \end{aligned} \tag{2.3.1}$$

It follows that [11]

$$\omega := \langle\rho(t)\rangle_\infty = \$_H(\rho(0)) \tag{2.3.2}$$

is a proper density matrix. Here $\$_H$ is the dephasing map with respect to H, acting as

$$\rho \longmapsto \$_H(\rho) := \sum_{E_n} P_{E_n}\rho P_{E_n}. \tag{2.3.3}$$

Using the special basis introduced in eq. 2.2.13, one has

$$\omega = \sum_{E_n, r_j} \rho_{E_n, r_j E_n, r_j}(0) |E_n, r_j\rangle\langle E_n, r_j| = \sum_{E_n, r_j} p_{E_n, r_j} |E_n, r_j\rangle\langle E_n, r_j| \quad (2.3.4)$$

Analogously, we define time averages for expectation values of observables A as

$$\langle\langle A\rangle_{\rho(t)}\rangle_T := \frac{1}{T}\int_0^T \langle A\rangle_{\rho(t)} dt. \quad (2.3.5)$$

One then obtains

$$\langle\langle A\rangle_{\rho(t)}\rangle_\infty = \mathrm{Tr}\{\omega A\} \quad (2.3.6)$$

In order to properly formalize the above mentioned concept of equilibration for expectation values, it is crucial to study how much these deviate from the time average for each individual time t. That is, one has to find out whether the quantity

$$\sigma(t) := \mathrm{Tr}\{\rho(t)A\} - Tr\{\omega A\} \quad (2.3.7)$$

is small for the majority of times t in any sufficiently large time interval $[0, T]$. By small we mean, in a realistic situation, that $|\sigma(t)| \ll \delta A$.

To determine the smallness of $\sigma(t)$ for most times one has to look at the variance

$$\sigma_A^2(T) := \langle\sigma^2(t)\rangle_T. \quad (2.3.8)$$

Viewing $\sigma^2(t)$ as a random variable, one can invoke the *Chebyshev* inequality, which states that for any random variable x with mean value μ and variance σ^2 and any given $\kappa > 0$, the probability that x deviates from μ by more than κ satisfies $Prob(|x - \mu| \geq \kappa) \leq (\sigma/\kappa)^2$. Applied to $\sigma^2(t)$ one gets

$$Prob(|Tr\{\rho(t)A\} - Tr\{\omega A\}| \geq \delta A) := \frac{T_{\delta A}}{T} \leq \frac{\sigma_A^2}{\delta A^2} \quad (2.3.9)$$

where

$$T_{\delta A} := |\{0 < t < T : |Tr\{\rho(t)A\} - Tr\{\omega A\}| \geq \delta A\}| \quad (2.3.10)$$

denotes the measure ($|S|$ is the *Lebesgue* measure of the set S) of all the times $t \in [0, T]$ for which $|\sigma(t)| \geq \delta A$ holds true. If σ_A is small, one can infer from this the smallness of $T_{\delta A}$, which means that the conditions for equilibration of expectation values of A have been fulfilled.

It is important to keep in mind that it is the existence of the finite resolution δA which makes this concept of equilibration compatible with the quantum mechanical time evolution. If one was able to measure with any accuracy, arbitrarily small fluctuations could be resolved and the system could never spend most of the time close to equilibrium, i.e. equilibration would lose its meaning. One also sees the compatibility with time-reversal symmetry. Non-equilibrium situations happen to be just these very short excursions (for sufficiently large total time intervals) away from the average.

2.3.2 Distinguishability

The fact that the difference in expectation values of an observable between $\rho(t)$ and ω is smaller than the minimal resolution of course does not imply that the two states cannot be distinguished. Especially it does not mean that the system as a whole has equilibrated, as usually assumed in ordinary statistical mechanics. It is, for example, possible that they yield different probabilities for different measurement outcomes, despite giving the same expectation value. More generally one can ask how to distinguish two states by a general measurement M represented by a POVM. This leads to the so called *distinguishability* of quantum states by measurement [20]. It can be motivated in the following way.

Suppose you are given with equal probability one of the two states ρ_1 and ρ_2 and you have to tell which of the two it is by performing the measurement M. The maximum success probability p_M^{max} corresponds to choosing for each measurement outcome of M the state which has the higher probability for that outcome. This can be calculated to give

$$p_M^{max} = \frac{1}{2}(1 + D_M(\rho_1, \rho_2)), \tag{2.3.11}$$

where $D_M(\rho_1, \rho_2)$ is the aforementioned distinguishability of ρ_1 and ρ_2 using measurement M, given by

$$D_M(\rho_1, \rho_2) := \frac{1}{2}\sum_a |Tr\{\rho_1 M_a\} - Tr\{\rho_2 M_a\}|. \tag{2.3.12}$$

In the case of a set of measurements $\mathcal{M}$ we define

$$D_{\mathcal{M}}(\rho_1, \rho_2) := \max_{M \in \mathcal{M}} D_M(\rho_1, \rho_2). \tag{2.3.13}$$

The distinguishability with respect to $\mathcal{M}$ is symmetric in its arguments and satisfies the triangle inequality. If $\rho_1 = \rho_2$ it is equal 0. However even if the two states are not equal $D_{\mathcal{M}}(\rho_1, \rho_2)$ can vanish, i.e. it does not define a proper metric. This is not surprising since one particular set of measurements might simply be not good enough to distinguish them. There is however always an optimal measurement, which is a two-outcome projective measurement onto the positive and negative eigenspaces of $\rho_1 - \rho_2$ [12]. The distinguishability with respect to that measurement is given by the *trace-distance*

$$D(\rho_1, \rho_2) := \frac{1}{2}Tr\{|\rho_1 - \rho_2|\}, \tag{2.3.14}$$

where $|\rho| := \sqrt{\rho^\dagger \rho}$. It is equal to the case when $\mathcal{M}$ corresponds to the set of all measurements and we have

$$0 \leq D_{\mathcal{M}}(\rho_1, \rho_2) \leq D(\rho_1, \rho_2) \leq 1. \tag{2.3.15}$$

The trace distance defines a proper metric with the property that $D(\rho_1, \rho_2) = 0 \Leftrightarrow \rho_1 = \rho_2$ and as such can always be used two distinguish any two states.

During the time evolution of a system usually no single measurement will be able to distinguish the current state from the equilibrium state for most times. One will have to use different measurements at different times. However especially for macroscopic systems with huge dimensions of $\mathcal{H}$ the realistic number of possible measurements $\mathcal{M}$ will be very limited, normally it will be finite. As such, the trace distance is of little use here.

Taking such a set of measurements one can define *equilibration to a state* σ *over the time interval* $[0, T]$ *with respect to* $\mathcal{M}$, if and only if

$$\langle D_{\mathcal{M}}(\rho(t), \sigma)\rangle_T \ll 1. \tag{2.3.16}$$

Since $D_{\mathcal{M}}(\rho(t), \sigma)$ is a non-negative number for all t, then if $\langle D_{\mathcal{M}}(\rho(t), \sigma)\rangle_T$ is small, $D_{\mathcal{M}}(\rho(t), \sigma)$ must be small for most of the time.

2.3.3 Results on equilibration

We will now give the known strongest general results on the equilibration of expectation values and equilibration with respect to measurement outcomes. First two important definitions are necessary.

The first concerns differences in the d' unique energy values. Every energy gap $E_i - E_j$ can be labelled by an ordered pair of integers i, j with $i \neq j$. One can now define the *set of energy gaps* $\mathcal{G}$ by

$$\mathcal{G} = \{(i, j) : i, j \in \{1, 2, ...d'\}, i \neq j\} \tag{2.3.17}$$

There are $d'(d'-1)$ energy gaps, some of which can be degenerate. We say $N(\varepsilon)$ is the maximum number of energy gaps in any energy interval of length ε, i.e. (using the notation $G_\alpha = E_i - E_j$ for $\alpha = (i, j)$)

$$N(\varepsilon) := \max_E |\{\alpha : \alpha \in \mathcal{G}, G_\alpha \in [E, E + \varepsilon]\}|. \tag{2.3.18}$$

The maximum number D_G of energy gaps is given by

$$D_G = \lim_{\varepsilon \to 0} N(\varepsilon), \tag{2.3.19}$$

while $D_G = 1$ corresponds to the non-degenerate gaps condition.

The second definition concerns the number of energy eigenstates that are populated by the initial state $\rho(0)$. For every such state we define the *effective dimension* as

$$d_{\text{eff}} := \frac{1}{\sum_{E_n} (Tr\{\rho(0) P_{E_n}\})^2}. \tag{2.3.20}$$

It follows that $1 \leqslant d_{\text{eff}} \leqslant d'$ and $d_{\text{eff}} = N$, when the state is spread equally over N different energy levels. The motivation behind this definition is, that states which are superpositions of a small number (but larger than 1) of energy states, have small d_{eff}. This leads to strong oscillatory behaviour in time for observable expectation values, reminiscent of *Rabi-oscillations* and prevents equilibration. As we have seen in 2.2.2, realistic initial states have large effective dimensions.

The relation $d_{\text{eff}}(\max_{E_n}\ p_{E_n}) \geqslant 1$ always holds. However, as we will see, it will prove sufficient for equilibration that $\max'_{E_n}\ p_{E_n}$, the second largest level occupation, is small.

We will now state the general results on equilibration in the form of two theorems ([11], [12], [10], see also [13] for earlier results, a partial proof can be found in the appendix).

Theorem 1: *(equilibration of expectation values) Let $\rho(0)$ be the initial state, ω the time-averaged state, p_{E_n} the energy level occupations of $\rho(0)$ and A the observable to be measured (all defined as above). Then, for every $\varepsilon > 0$ and every time interval $[0, T]$ it holds that*

$$\sigma_A^2(T) \leq ||A||_\infty^2 N(\varepsilon) f(\varepsilon\, T) g((p_{E_n})_1^{d'}), \tag{2.3.21}$$

where $||A||_\infty$ is the operator norm of A and

$$\begin{aligned} f(\varepsilon\, T) &:= 1 + \frac{8\ \log_2 d'}{\varepsilon\, T} \\ g((p_{E_n})_1^{d'}) &:= \min\,(\frac{1}{d_{\text{eff}}}, 3 \max_{E_n}{}' p_{E_n}). \end{aligned} \tag{2.3.22}$$

Theorem 2: *(equilibration with respect to measurement outcomes) With the same notation as in theorem 1, let $\mathcal{M}$ represent a set of measurements, then*

$$\langle D_{\mathcal{M}}(\rho(t), \omega)\rangle_T \leq \mathcal{S}(\mathcal{M})(N(\varepsilon) f(\varepsilon\, T) g((p_{E_n})_1^{d'}))^{1/2}, \tag{2.3.23}$$

where

$$\mathcal{S}(\mathcal{M}) := \min(|\cup\mathcal{M}|/4, \dim \mathcal{H}_{\text{supp}(\mathcal{M})}/2), \tag{2.3.24}$$

with $\cup\mathcal{M}$ the set of all distinct POVM elements in $\mathcal{M}$, and $\text{supp}(\mathcal{M}) := \bigcup_{M\in\cup\mathcal{M}} \text{supp}(M)$.

As discussed in 2.2.2, the quantity $g((p_{E_n})_1^{d'})$ is small under reasonably realistic conditions. The quantity $\mathcal{S}(\mathcal{M})$ can be assumed to be much smaller than d'. If then the number of energy gaps is not too large, these theorems imply equilibration under reasonable restrictions on measurements for large enough

time intervals.

It is also possible to express these results in terms of Δ_A and δA. By setting ε equal to the minimum spacing between non-degenerate energy gaps, i.e.

$$\varepsilon = \varepsilon_{\min} := \min\{|G_\alpha - G_\beta| : G_\alpha \neq G_\beta\}, \tag{2.3.25}$$

one sees, using eq. 2.3.19, that $N(\varepsilon_{\min}) = D_G$. One can then make T sufficiently large such that $N(\varepsilon) f(\varepsilon\, T) \leq 2D_G$. Finally replacing A by $A + c\, Id$, where c is a real number, leaves $\sigma(t)$ unchanged. Choosing c so that $a_{max} = -a_{min}$, it follows that $||A||_\infty = \Delta_A/2$. From this one can deduce, using eq. 2.3.9, that

$$\frac{T_{\delta A}}{T} \leq \frac{1}{2} D_G (\frac{\Delta_A}{\delta A})^2 g((p_{E_n})_1^{d'}) \tag{2.3.26}$$

for all sufficiently large T.

In the case where the support of $\mathcal{M}$ is contained in a subsystem of the whole system, $\mathcal{S}(\mathcal{M})$ is bounded by $d_s/2$, where d_s is the dimension of the subsystem. One then obtains the remarkable result that

$$\langle D(\rho_s(t), \omega_s)\rangle_T \leq \frac{1}{2} (d_s^2 N(\varepsilon) f(\varepsilon\, T) g((p_{E_n})_1^{d'}))^{1/2}, \tag{2.3.27}$$

where $\rho_s(t)$ is the reduced state of $\rho(t)$ and $\omega_s = \langle \rho_s(t)\rangle_\infty$. If $d_s^2 \gg g((p_{E_n})_1^{d'})$, subsystem equilibration with respect to any measurement follows. However, as opposed to the results on the whole system, the equilibration of the subsystem is not a consequence of our experimental limitations (on $\mathcal{M}$ and δA), but an objective property, since it is valid for all measurements on the subsystem.

2.3.4 Time scales for equilibration

So far we have inferred only the existence of equilibration, but not the time scale on which it occurs. First, the uncertainty between H and A gives a basic minimum time scale on which equilibration can happen [14]. This follows from $2\sigma_E \sigma_A \geq |\langle [H, A]\rangle| = |\langle \dot{A}\rangle|$, where σ_E is the energy uncertainty and σ_A the uncertainty of the observable A in the initial state $\rho(0)$. Transforming these inequalities one defines the time scale

$$t_{\min} := \frac{\sigma_A}{|\langle \dot{A}\rangle|} \geq \frac{1}{2\sigma_E}. \tag{2.3.28}$$

The time scale $1/\sigma_E$ (recall that $\hbar = 1$) corresponds to the minimal time such that one observes significant variations in the observable A. As such it is also the minimal time to observe equilibration.

We can now use the formulas from theorems 1 and 2 to derive lower bounds $\mathrm{T}_{\min}$ on equilibration times together with their scaling properties. This means that all the system fulfilling the conditions of the theorems will have definitely

equilibrated after this time. However they might already have done so after a much shorter time. $\mathrm{T}_{\min}$ can then be compared to $t_{\min}$ [14].

First we choose ε such that $N(\varepsilon) \leq d_{\text{eff}}$. $N(\varepsilon)$ is bounded by $d'(d'-1)$, the number of energy gaps, and has its minimum at $\varepsilon = \varepsilon_{\min}$. Assuming that the eigenvalues of the Hamiltonian are reasonably evenly distributed over the energy width of the initial state ΔE, one can expect that the optimal value is $\varepsilon = \eta \frac{\Delta E}{d'}$, where $\eta \ll 1$. We then deduce from 2.3.23, that equilibration will occur as long as

$$\mathrm{T}_{\min} \gtrsim \frac{\log_2 d'}{\varepsilon} = \frac{d' \log_2 d'}{\eta \Delta E}. \tag{2.3.29}$$

This means that in general equilibration times scale roughly as $\dfrac{d'}{\Delta E}$. This corresponds to a scaling that is linear in the dimension d', and as such exponential in the number of degrees of freedom f. Even though this is much shorter than the recurrence time, which scales exponentially in d', it is huge (it easily exceeds the age of the universe) compared to the very short time scale $t_{\min}$.

One might first be inclined to view this time as far too long (unphysical) and so the bound as too rough. However one has to keep in mind that the conditions for theorem 1 and 2 are very general. It is indeed possible to find systems and measurements, which fulfill these conditions, having such long equilibration times [14]. This then means that a smaller bound requires a stronger restriction on the Hamiltonian or the measurements. So far almost all systems for which equilibration in the sense as we have defined it has been shown in numerical simulations, have reasonable time scales. The lower bound is then not very tight for them.

Basically all the analytical results, which go beyond these theorems, have the form of *typicality* theorems ([14],[15],[16],[17]). They prove reasonable equilibration times for all but a few Hamiltonians from certain probability measures, but cannot be applied to any concrete Hamiltonian. Usually the time scales are very short, of the order of $t_{\min}$, which begs the question why equilibration times of known systems are often longer (for example cooling of hot coffee at room temperature [15]).

2.4 Thermalization

2.4.1 General definition

After defining what it means for a quantum system to equilibrate in the previous chapters, we are now ready to ask the question whether and in what sense such a system behaves thermally. We have described in the previous chapter equilibrium states through the diagonal ensemble $\$_H(\rho(0))$. However, this state depends on the initial state $\rho(0)$. This does not agree with the concept that we have of a thermal state which should be largely independent of the initial con-

dition. So in order to speak of thermalisation, $\$_H(\rho(0))$ must somehow be close to a thermal state. This will lead us again to the concept of distinguishability of states with respect to general measurements.
We will now first described what we see as general conditions for thermalization of a quantum system [11].

- *Equilibration*: The system must equilibrate with respect to some set of measurements $\mathcal{M}$ or expectation values of observables $\mathcal{A}$ in the sense described in the last chapter. This includes also the case where only a subsystem of the whole system equilibrates.
- *Independence of the initial state*: The equilibrium state should depend only on some macroscopic properties like the mean energy density of the initial state for at least a large class of initial states. In the case of subsystem thermalization this should apply to both the initial states of the subsystem and the bath.
- *Close to a thermal state*: We mean by thermal states one of the statistical ensembles defined in section 2.2.6, namely the microcanonical, the Gibbs- and generalized Gibbs ensemble. In the case of the microcanonical ensemble one expects its applicability only in the case where the energy width ΔE of the initial state is very small. The generalized Gibbs ensemble is usually only considered as being thermal when the number of conserved quantities grows slowly (i.e. slower than the dimension of the Hilbert space of the system) with the system size (see section 2.5). Otherwise one could hardly speak of initial state independence.

From these conditions we distil, using the concepts introduced in the previous chapters, the following general definition of thermalization [11]. We will only consider the microcanonical and canonical ensembles.

Thermalization with respect to measurements:

We say that a system with Hamiltonian H thermalizes with respect to a set of generalized measurements $\mathcal{M}$ for a set of initial states $\mathcal{S}_0$, if for each $\rho_0 \in \mathcal{S}_0$ it equilibrates to $\omega = \$_H(\rho_0)$ and $\mathcal{D}_{\mathcal{M}}(\omega, \rho_{th})$ *is sufficiently small. Here ρ_{th} means either $\rho_{mc}[H](E, \Delta)$ or $\rho_G[\tilde{H}](\beta(\mathrm{Tr}\{H\rho_0\}))$, where (E, Δ) are the mean energy and energy width of ρ_0 and $\tilde{H}$ is some Hamiltonian. This definition implicitly also defines thermalization for subsystems.*

Thermalization with respect to expectation values:

We say that a system with Hamiltonian H thermalizes with respect to expectation values of observables $\mathcal{A}$ for a set of initial states $\mathcal{S}_0$, if for each $\rho_0 \in \mathcal{S}_0$ it equilibrates to $\omega = \$_H(\rho_0)$ and for each $A \in \mathcal{A}$ the difference $|\langle A\rangle_\omega - \langle A\rangle_{\rho_{th}}|$ is sufficiently small, where small usually means smaller than δA. Also the fluctuations around the expectation value are required to be small in the thermodynamic limit.

2.4.2 Eigenstate thermalization hypothesis

After this general definition the question raises how to determine whether a concrete system thermalizes or not. Is there some necessary and sufficient condition for thermalization?
In attempting to answer this question one concept that has become popular in recent years is the so called *Eigenstate thermalization hypothesis* (ETH) ([5],[25],[28],[31]). It is a condition on the eigenstates of a system. In its simplest form it can be defined as follows [5]

Suppose that a system with Hamiltonian $H = \sum_{E_n} E_n P_{E_n}$ (we are using the special basis $|E_n, r_j\rangle$ defined in eq. 2.2.13) and initial state ρ_0 equilibrates with respect to the expectation value of some observable A. The equilibrium state is then, according to eq. 2.3.6, $\omega = \sum_{E_n,r_j} p_{E_n,r_j} P_{E_n,r_j}$. The equilibrium expectation value of A is given by

$$\mathrm{Tr}\{A\omega\} = \sum_{E_n,r_j} p_{E_n,r_j}\langle E_n, r_j|A|E_n, r_j\rangle \;=\; \sum_{k=1}^{\dim(\mathcal{H}_{E,\Delta})} p_k\langle k|A|k\rangle \;, \qquad (2.4.1)$$

where we have changed the notation for the basis states $|E_n, r_j\rangle$ to $|k\rangle$, assuming that $p_k \neq 0$ only in some narrow energy interval $I_{E,\Delta}$. For thermalization to happen, eq. 2.4.1 must be close to the expectation value of A in a thermal state. We can compare the above expression with the expectation value of A in the microcanonical state defined on that energy interval, $\rho_{\mathrm{mc}}[H](E, \Delta)$:

$$\mathrm{Tr}\{A\rho_{\mathrm{mc}}\} = \frac{1}{\dim(\mathcal{H}_{E,\Delta})} \sum_{k=1}^{\dim(\mathcal{H}_{E,\Delta})} \langle k|A|k\rangle \;, \qquad (2.4.2)$$

Under which conditions on H, ρ_0 and A could these two expressions be very close in value? Basically three different possibilities suggest itself [5]

- *unbiased sampling*: Both the expectation values $\langle k|A|k\rangle$ and the probabilities p_k will have large fluctuations even for states close in energy. However for physically interesting initial conditions the fluctuations of these

two quantities are uncorrelated. Equation 2.4.1 then basically corresponds to an unbiased sampling of $\langle k|A|k\rangle$. This is equal to eq. 2.4.2.

- *equal probabilities*: For physically interesting initial conditions the probabilities p_k are almost equal for eigenstates close in energy. Equality of 2.4.1 and 2.4.2 then follows.

- *ETH*: The ETH states that $\langle k|A|k\rangle$ is a smooth function of the energy eigenstates $|k\rangle$ (or any other energy eigenstates). Again equality of the two expressions follows, if all eigenstates $|k\rangle$ are close in energy. In that case it holds for all initial states with a sufficiently small energy width, unlike in the other two scenarios. There particular states could violate the assumptions.
  It then follows that the expectation value of A in any of the energy eigenstates $|k\rangle$ is approximately equal to a thermal expectation value:

$$\langle k|A|k\rangle \approx \langle A\rangle_{\rho_{\mathrm{mc}}} \tag{2.4.3}$$

  This is where the name eigenstate thermalization comes from.

Because of their strong dependence on particular properties of the initial state, the first two scenarios can hardly present general mechanisms for thermalization. Especially the second one can be basically ruled out. According to the discussion in 2.2.4, the assumption of equal probabilities is violated by the form of experimentally realistic initial states in closed system experiments.
This leaves us with the ETH. Using again the concept of distinguishability of states with respect to measurements, it is possible to give a more general and precise definition of the ETH [11].

ETH with respect to measurements:

Let H be some Hamiltonian and I some energy interval. We denote by S the set of all eigenenergies E_k of H, with $E_k \in I$. Let $\mathcal{H}_{E_k}$ be the projective subspace of P_{E_k}. We say that H fulfils the eigenstate thermalization hypothesis in I with respect to the set of measurements $\mathcal{M}$, if for every $E_k \in S$ and for every normalized pure state $\psi \in \mathcal{H}_{E_k}$ the distinguishability $\mathcal{D}_{\mathcal{M}}(\psi, \rho_{th}(E_k))$ is sufficiently small. Here $\rho_{th}(E_k)$ is either $\rho_{mc}[H](E_k, \Delta)$, with Δ small such that $I_{E,\Delta} \subset I$. Or ρ_{th} is equal to $\rho_G[H](\beta(E_k))$, where β is some smooth function $I \to \mathbb{R}^+$.

ETH with respect to expectation values:

Let H be some Hamiltonian and I some energy interval. We denote by S the set of all eigenenergies E_k of H, with $E_k \in I$. Let $\mathcal{H}_{E_k}$ be the projective subspace of P_{E_k}. Let $\mathcal{A}$ be a set of observables. We say that H fulfils the eigenstate thermalization hypothesis in I with respect to the expectation values of $\mathcal{A}$, if for every $A \in \mathcal{A}$, for every $E_k \in S$ and for every normalized pure state $\psi \in \mathcal{H}_{E_k}$ the difference $|\langle\psi|A|\psi\rangle - \langle A\rangle_{\rho_{th}(E_k)}|$ is sufficiently small. Here $\rho_{th}(E_k)$ is either $\rho_{mc}[H](E_k, \Delta)$, with Δ small such that $I_{E,\Delta} \subset I$. Or ρ_{th} is equal to $\rho_G[H](\beta(E_k))$, where β is some smooth function $I \to \mathbb{R}^+$. Sufficiently small means again usually smaller than δA.

In the case where the energy interval I is very narrow, ρ_{th} corresponds basically to just one $\rho_{mc}[H](E, \Delta)$ in the microcanonical scenario while β is basically constant in the canonical scenario. In each case there is just one thermal state. Every initial state, which has an energy distributions entirely contained in I and which equilibrates, does so to $\$_H(\rho(0))$, which has the form defined in equation 2.3.4 and as such is diagonal in the eigenstates of H. From the triangle inequality for the distinguishability with respect to $\mathcal{M}$ (respectively from the triangle inequality for absolute values of real numbers in the case of expectation values), thermalization in the sense of definition 2.4.1 then follows from the ETH for all such initial states.

There is a second part of the ETH which gives a condition on the equilibration of the system in the diagonal ensemble ([26], [27]). To formulate it we can use the concepts developed in the section on equilibration. In a general energy eigenbasis, under the assumption of the non-degenerate energy gaps condition (see section 2.2.1), the squared variance $\sigma_A^2(T \to \infty)$ can be written as

$$\sigma_A^2(T \to \infty) = \sum_{E_n \neq E_m} p_{E_n} p_{E_m} |A_{nm}|^2 \tag{2.4.4}$$

In order to guarantee the smallness of the right hand side of eq. 2.4.4 for general initial states (recall that Theorem 1 gives an upper bound), the second part of the ETH imposes that the absolute values of the off diagonal matrix elements $|A_{nm}|$ are small. More exactly $|A_{nm}|$ should be exponentially small in the system size. In section 3 we are going to see that this is indeed the case for the Systems used in our numerical studies.

The ETH can then be seen as a sufficient condition for thermalization. Is it also necessary? The intuition seems to suggest that it is also a necessary condition. If the ETH is not satisfied then there exist eigenstates of H which can be distinguished from thermal states by some measurements. Taking some initial state which has an overlap with such eigenstates, the distinguishability should

then also be seen in the dephased state and hence survive equilibration [11].

The question is now how to test the ETH. If one cannot give strong general criteria how to test it, then one could argue that one has replaced one poorly understood problem, namely thermalization, by another poorly understood phenomenon [23].
So far the ETH has been shown to be true mainly in numerical studies of relatively small (up to about 25 sites) systems of particles or spins ([5],[25],[60],[63], [64],[65]). This was done usually by exact numerical diagonalization or finite size scaling. Rigorous analytical result exist so far only for systems with very special Hamiltonians [29].
In [28] thermalisation of the momentum distribution numbers via the ETH was shown for a system which is the quantisation of the classical hard sphere gas. The result is based on the *Berry conjecture* [59], which is a statement about the eigenstates of quantum systems whose classical counterparts exhibit chaotic behaviour (classically non integrable models like the hard sphere gas). Similar ideas based on random Hamiltonians were considered in [31] (see also [33] and [32]).
One can ask whether there is some intuitive argument that explains which are the particular measurements that satisfy (or violate) the ETH in the case of eigenstates of a particular Hamiltonian. Looking for example at the expectation value version of the ETH, how can an observable that satisfies the hypothesis tell that two eigenstates are close in energy [33]?
In general it is clear, that the ETH cannot be fulfilled for all observables for any particular Hamiltonian [33]. Taking an observable A with matrix elements in the energy basis $|n\rangle$, defined as $A_{nn} = (-1)^n$ and A_{nm} arbitrary for $n \neq m$. This observable certainly violates the ETH in any energy interval. It is of course another question whether this so defined observable represents any experimentally measurable quantity. We will later see that there are currently two known classes of system, for which observables can be found, that violate the ETH. The integrable systems and the many body localised systems.
One problem with our intuition about the ETH seems to be that we usually think about observables as one particle observables, like kinetic energy, density or magnetisation. This is so because our intuition is strongly based on thinking in terms of individual particles (or spins) ([34], [46]). These observables are exactly the ones which have eigenstates that are products of single particle states. Non interacting systems have these states as their eigenstates and they violate the ETH. They are special cases of the above mentioned integrable models.
However, a generic Hamiltonian has interactions and its eigenstates have in general no special relation to that of a generic observable A. We have already seen in our discussion of perturbation theory in section 2.2.6 that even a small perturbation of a Hamiltonian, like a small interaction among particles, changes drastically the eigenstates with respect to the original unperturbed eigenbasis because of the huge number of states that are close in energy. The eigenstates become randomized with respect to the non interacting ones and as such also with respect to the one particle observables. In this way neighbouring levels

become similar to each other and as such one could see this as a first hint to the ETH.

2.4.3 Typicality

In the previous chapters we have formulated the general concept of thermalization in the terms of the distinguishability of states with respect to measurements and expectation values. We have introduced the eigenstate thermalization hypothesis and given arguments for it to be a necessary and sufficient condition for thermalization. However, we also noted that general proofs of the ETH are lacking.

The concept of *typicality*, which we will discuss in this chapter, can shed new light on both thermalization and the ETH. It is based on the idea that a certain property (like thermalization) might be, in a way to be defined precisely, a typical property of quantum systems. As a first example, in *random matrix theory* [35] one studies the properties of a particular (probably not exactly known) Hamiltonian by looking instead at a whole ensemble of Hamiltonians and averages over the properties of them. In the case where most Hamiltonians have the same property, this might give a meaningful result even for the particular system one is interested in. This method has proven very successful in the study of the spectra of complex nuclei.

In order to properly define the notion of most, we use the language of probability theory. In particular we will need the concept of a probability measure. The one that we will use here is the uniform *Haar measure*. It is the unique, left/right invariant, countably additive, normalized measure on the group $U(d)$ of unitary transformations of a d-dimensional Hilbert space $\mathcal{H}$ [11], and we denote it by $\mu_{\text{Haar}}[U(d)]$. Left/right invariant means that for any unitary $U \in U(d)$ and any Borel set $\mathcal{B} \subseteq U(d)$

$$\mu_{\text{Haar}}[U(d)](\mathcal{B}) = \mu_{\text{Haar}}[U(d)](U\mathcal{B}) = \mu_{\text{Haar}}[U(d)](\mathcal{B}U), \tag{2.4.5}$$

where $U\mathcal{B}$ and $\mathcal{B}U$ are the left and right translates of $\mathcal{B}$. It is this property why the Haar measure is called the uniform measure on $U(d)$. One obtains from the Haar measure a probability distribution (the uniform distribution) over the set of orthonormal basis of $\mathcal{H}$. This is done by first fixing any particular orthonormal basis. Applying the random-Haar distributed U's to the basis vectors one gets a Haar-random orthonormal basis. The marginal distribution of any fixed basis vector defines the uniform distribution on the unit sphere of physical states of $\mathcal{H}$. We call states drawn according to this measure Haar-random. In an analogous way the Haar measure can be extended from orthonormal basis to Hamiltonians and observables.

Before applying typicality to our problems of thermalization, in order to avoid crucial misunderstandings, we want to first address some of the general criticism that this method has faced in the past [37].

It has been argued that the assignment of equal probabilities to for example observables is physically unjustified because in reality it is not possible to measure every observable. While this is certainly correct, the usage of the language of probability theory in the method of typicality is only a formally elegant tool to obtain information about the sizes of certain sets (of states, Hamiltonians,...). So one in reality does not use random objects, like for example the above mentioned random matrices, but looks for behaviour that is typical among different systems. If some condition is shown to be true for most states (Hamiltonians, observables,...), than this suggests that it might also be true for some given concrete system, unless we have reasons to expect otherwise. Of course this does not prove that the condition is really true for the given system, this can only be done by checking it directly. But to know which behaviour is typical and which is exceptional might be a very useful information.

Generally, the greater the degree of certainty a typicality theorem confers, the smaller is its explanatory power. This shall be illustrated on an example [37]. Let the Hamiltonian H belong to some subset S_0 of the set S of all self-adjoint operators on $\mathcal{H}$. There are in principal two typicality theorems of interest. One says the the relevant behaviour occurs for most $H \in S_0$, the other that it is true for most $H \in S$.
When S_0 is very small compared to S, the two statements are logically independent. However, each statement has its own merits: The first theorem gives us a greater certainty that the relevant behaviour will occur for the given Hamiltonian H. The second theorem tells us that the relevant behaviour has not much to do with S_0 but is widespread all over S. As such it has greater power in explaining why the property occurs.

Generalization of Von Neumann's approach:

In section 4.2 we describe Von Neumann's typicality. One weakness of this approach to thermalization is that it applies only to macroscopic observables. However experiments and numerical simulations have established that the applicability of statistical mechanics is far greater than that (one well know classic example is Brownian motion). Very recently Von Neumann's approach to thermalization has been generalized in ref. [46]. The established typicality results apply to general observables and to general initial states, including mixed states. The only prerequisite is for the Hamiltonian to fulfil the non-degenerate energy gaps condition (and as such especially no degenerate eigenvalues).

Considering now one such Hamiltonian H and some arbitrary observable A, we denote by U the unitary transformation between the eigenstates of H and A. The time averaged deviation

$$\sigma_A^2(T) := \langle(\langle A\rangle_{\rho(t)} - \langle A\rangle_\omega)^2\rangle_T \tag{2.4.6}$$

where $\omega := \langle\rho(t)\rangle_\infty = \$_H(\rho(0))$ is the infinite time averaged state (see section

2.3.1) satisfies the following relation in the limit $T \to \infty$:

$$\begin{aligned}
\sigma_A^2(\infty) &= \sum_{m \neq n}^{D} |\rho_{mn}(0)|^2 |A_{mn}|^2 \\
&\leqslant \sum_{m \neq n}^{D} |\rho_{mn}(0)|^2 \max_{m \neq n} |A_{mn}|^2 \\
&\leqslant \sum_{m \neq n}^{D} |\rho_{nn}(0)|^2 |\rho_{mm}(0)|^2 \max_{m \neq n} |A_{mn}|^2 \\
&\leqslant \sum_{m}^{D} |\rho_{mm}(0)|^2 \max_{m \neq n} |A_{mn}|^2 = \max_{m \neq n} |A_{mn}|^2.
\end{aligned} \tag{2.4.7}$$

For the step from the second to the third line the Cauchy-Schwartz inequality for the scalar product

$$(n, m) := \rho_{nm}(0) = \langle n|\rho(0)|m\rangle \tag{2.4.8}$$

has been used. It follows from this inequality that equilibration, measured by σ_A^2, is linked to the smallness of the off diagonal elements of the observable A in the energy eigenbasis. This corresponds to the second part of the eigenstate thermalization hypothesis discussed in section 2.4.2. In [46] it is shown that these matrix elements are so small that

$$\mu_U(\sigma_A^2(\infty)) \geq \varepsilon) \leq 4 \exp(-\frac{\varepsilon D}{18\pi^3 \Delta_A^2} + 2 \ln D) \tag{2.4.9}$$

for any $\varepsilon > 0$, where μ_U is again the uniform measure on the unit sphere in $\mathcal{H}$. The main ingredient in the derivation of eq. 2.4.9 is the so called *Levy's Lemma* (see [47], [48]). It is a statement about the statistical properties of functions which are defined on the d-dimensional unit sphere $\mathcal{S}^d$ in $\mathbb{R}^{d+1}$. More preciselly it states that

$$\text{Prob}(|g(\phi) - \langle g\rangle| \geq \varepsilon) \leq 2 \exp(-\frac{\varepsilon^2 (d+1)}{9\pi^3 \eta^2}) \tag{2.4.10}$$

for randomly and uniformly distributed points ϕ on $\mathcal{S}^d$ and g is a *Lipschitz continuous* function $\mathcal{S}^d \to \mathbb{R}$ with Lipschitz constant η and mean value $\langle g\rangle$. Any $|\phi\rangle = \sum_n c_n |n\rangle$, where $|n\rangle$ is a complete set of energy eigenstates, can be represented as a point ϕ on the $(2D-1)$-dimensional unit sphere via it's real and imaginary parts. Levy's Lemma can then be applied to the function $g(\phi) := \langle \phi|A|\phi\rangle$ which is shown to be Lipschitz continuous with $\eta = \Delta_A$ in reference [48]. The fact that $\langle g\rangle = \langle A\rangle_{\rho_{\text{mc}}}$ has been proven in 4.2.8. Since randomizing ϕ is equivalent to randomizing the unitary U, one thus obtains

$$\mu_U(|\langle \phi|A|\phi\rangle - \langle A\rangle_{\rho_{\text{mc}}}| \geq \varepsilon) \leq 2 \exp(-\frac{2\varepsilon^2 D}{9\pi^3 \eta^2}) \tag{2.4.11}$$

for any $\varepsilon > 0$. From this the desired result bout the maximal $|A_{mn}|$ can be derived (see [46]) such that eq. 2.4.9 follows. The important thing about this result is that it demonstrates equilibration for an arbitrary initial state $\rho(0)$ under the assumption that the relation U between H and A is typical. By choosing for example $\varepsilon = \delta A^2/\sqrt{D}$, which is much smaller than the resolution, the right hand side of eq. 2.4.9 becomes very small.

In order to demonstrate thermalization it is is still necessary to make sure that the difference between $\langle A\rangle_\omega$ and $\langle A\rangle_{\rho_{\mathrm{mc}}}$ is negligibly small. Defining the quantity

$$B := \langle A\rangle_\omega - \langle A\rangle_{\rho_{\mathrm{mc}}} = \sum_n \rho_{nn}(0)(A_{nn} - \langle A\rangle_{\rho_{\mathrm{mc}}}), \tag{2.4.12}$$

one has

$$|B| \leq \max_n |A_{nn} - \langle A\rangle_{\rho_{\mathrm{mc}}}| \tag{2.4.13}$$

This result is equivalent to first part of the ETH. Similarly to above, eq. 2.4.11 can now be used to prove ([46]) that the typical values of $|A_{nn} - \langle A\rangle_{\rho_{\mathrm{mc}}}|$ are so small such that

$$\mu_U(|B| \geq \varepsilon) \leq 2\exp(-\frac{2\varepsilon^2 D}{9\pi^3\Delta_A^2} + \ln D) \tag{2.4.14}$$

for any $\varepsilon > 0$. This results implies that for any pair H, A with a typical U the difference $|\langle A\rangle_\omega - \langle A\rangle_{\rho_{\mathrm{mc}}}|$ is smaller than the resolution limit δA, which corresponds to thermalization. It is again important to emphasize that the result is independent of the initial state $\rho(0)$. It now follows from eq. 2.4.9 and eq. 2.4.14 that the measure of U's which give rise to both equilibration and negligibly small $|B|$-values is close to unity. This corresponds to a generalization of Von Neumann's QET (normal typicality), which is only valid for macroscopic observables characterized by the decomposition $\mathcal{D}$ and for pure initial states.

It is also possible, using this approach, to infer about behaviour for finite time intervals. Defining now the unitary W as the mapping between the eigenstates of the initial state (represented by the density operator $\rho(0)$) and the observable A, we consider the quantity

$$\sigma^2_{\mathrm{mc}}(t) := (\langle A\rangle_{\rho(t)} - \langle A\rangle_{\mathrm{mc}})^2. \tag{2.4.15}$$

Similarly as before it can be shown ([46]) that

$$\mu_W(\sigma^2_{\mathrm{mc}}(t) \geq \varepsilon) \leq \frac{\Delta_A^2}{\varepsilon D}, \tag{2.4.16}$$

for arbitrary t and $\varepsilon > 0$, and that

$$\mu_W(\frac{1}{t_2 - t_1}\int_{t_1}^{t_2} \sigma^2_{\mathrm{mc}}(t)dt \geq \varepsilon) \leq \frac{\Delta_A^2}{\varepsilon D}, \tag{2.4.17}$$

for arbitrary $t_1 < t_2$ and $\varepsilon > 0$. It is important to note that while the right hand side of eq. 2.4.16 and eq. 2.4.17 is time independent, the set of W's on the left hand side in each case depends on t.
Considering the observable A as fixed the above two equations can be interpreted in the following way: for any Hamiltonian H, for any fixed time point t , $\langle A\rangle_{\rho(t)}$ yields almost the same value as $\langle A\rangle_{\mathrm{mc}}$ for most initial states $\rho(0)$. The same is true for almost all times t in any arbitrary time interval $[t_1, t_2]$. This means that non equilibrium initial conditions with respect to A are rare among all initial states, as they require a special "orientation" W of $\rho(0)$ against A.
Conversely when considering $\rho(0)$ as given, it follows from equations 2.4.16 and 2.4.17 that for any Hamiltonian H most observables A cannot distinguish $\rho(t)$ from ρ_{mc} at any fixed time t and also for almost all time from and arbitrary time interval $[t_1, t_2]$.
The viewpoint of taking H as fixed and requiring a generic constellation W of A and $\rho(0)$ has been taken in references ([49], [50], [51], see also the discussion in [37]). As such it only infers about thermalization for most initial states but not for all. In Von Neumann's approach and it's generalization in eq. 2.4.9 and eq. 2.4.14 a generic orientation U between H and is required but any $\rho(0)$ is admitted. Since non equilibrium initial states are special, it is this approach which can infer about thermalization in the sense of the normal typicality defined above.

2.5 Transition from integrability to quantum chaos

2.5.1 Motivation

It has been shown in numerical studies that that the transition away from integrability is often accompanied by a qualitative change in a system's properties other than thermal behaviour. Two of the most often studied quantities are *level spacing distributions* of energy levels and *delocalization measures* of energy eigenstates with respect to some basis. The changes in these quantities often go hand in hand with a switch from non-thermal to thermal behaviour in the sense of the ETH as one departs from integrability ([60], [61], [62]). This can be anticipated by considering that as the energy eigenstates become delocalized, neighbouring levels become similar to each other (see the discussion at the end of section 2.4.2). This is the apperent reason why delocalization measures are such good indicators of thermal behaviour. We will also see in section 3.5.1 and 2.5.4 that systems far from integrability behave in many ways like random matrices.
The original studies were performed on quantum systems which possess a classical analogue ([66], [67]). One then observed the above mentioned change in behaviour as the corresponding classical system changed from integrability to ergodicity (chaos). This is the reason for calling the above quantities *indicators of quantum chaos*. It was later found that analogous behaviour also occurrs in systems without a well defined classical limit.
There is a similar phenomenon in classical mechanics when integrability is broken by changing a system parameter. At a certain strength of the integrability breaking term the system starts showing ergodic behaviour. The important point is that this transition is sharp as there is a threshold (KAM-threshold [70]) at which the system properties change abruptly.
In contrast the finite quantum systems studied display a smooth transition from integrability to quantum chaos which again usually goes hand in hand with a smooth transition to thermal behaviour. As the change in properties normally scales with the system size across the transition, the question remains whether in the thermodynamic limit there is a sharp KAM-like threshold [71].
The sudy of delocalization measures was motivated by Berry's conjecture on eigenstates of quantum hard sphere gases mentioned in section 2.4.2. Analogous behaviour (both for level spacing statistics as well as delocalization measures) was also observed ([72], [73]) for disordered system as they switch from many body localisation to thermal behaviour. This is not surprising as integrable systems can be viewed as being localised in conserved mode-space (also often called quasi particle space)([74], [75]). However there is one important difference between integrability and MBL. Whereas the first is destroyed by the tiniest perturbation the second prevails up to some critical value.

We are now going to first give a precise definition of integrability in quantum mechanics and then introduce in more detail the above mentioned indicators of quantum chaos.

2.5.2 The concept of integrability in quantum mechanics

In classical mechanics, there is a clear and powerful concept of integrability of a Hamiltonian system based on the existence of a certain number of integrals of motion (conserved quantities) and the stability with respect to small perturbations of integrability by means of the KAM-theorem. In quantum mechanics the situation is far more confusing with various (partially inequivalent) notions of integrability being used [53]. We will not dwell on these matters here. The notion of integrability we will use for the study of thermalization is motivated by two convictions:

(i) That systems with a large number of conserved quantities do not thermalize in the sense of the eigenstate thermalization hypothesis, where thermal states correspond either to the microcanonical- or canonical ensemble.

(ii) That it is possible for such systems to thermalize if one uses the generalized Gibbs ensemble as alternative definition of a thermal state.

Following [53], we believe our definition of integrability fulfils the following fundamental criteria [53] of being

- unambiguous;
- it partitions all physical systems into inequivalent classes;
- different classes of systems show different physical behaviour.

We will now state our definition of integrability of quantum systems. For a more general and formal definition see [53].

Def.:(integrability) We call a system of size N with Hamiltonian H *quantum integrable*, if it possesses the following properties:

(i) There is a set of operators $\{I_k, k = 1, ..., n\}$ such that $[I_k, I_l] = 0$ for all $k, l = 1, .., n$ and the Hamiltonian H is one of these I_k's. This means that the I_k's are integrals of motion.

(ii) The operators in $\{I_k, k = 1, ..., n\}$ are algebraically independent.

(iii) The cardinality n of the set $\{I_k, k = 1, ..., n\}$ grows like $O(f(N))$ with the system size N. Here O denotes the Landau symbol and the function f is maximally sub exponential.

The property (iii) is the main difference to the most common definition of integrability used in the literature. It guarantees that the number of the conserved quantities I_k grows slower with increasing system size than the dimension D of the Hilbert space, which grows exponentially fast. The most common notion of integrability (and the one that mostly resembles the notion of integrability used for classical systems) requires the number of integrals of motion to be maximal, equal to D. However, in every system one always has the projectors $|n\rangle\langle n|$ to the energy eigenstates $|n\rangle$ which satisfy this definition of integrability. In this sense every system could be called integrable.

The other reason for us to abandon the usual concept of integrability and the one directly related to thermalization has to do with the convictions (i) and (ii) formulated above. First, it seems plausible (and is confirmed by numerical studies) that it is the large number of additional (to the $|n\rangle\langle n|$'s) conserved quantities what is responsible for integrable systems to fail to thermalize. This is due to the expected correlations between probabilities p_n and expectation values $\langle n|A|n\rangle$ of observables in the diagonal ensemble (see section 3.3).
Secondly, let us look back at the definition of the generalized Gibbs ensemble in section 2.2.6 in terms of the integrals of motion I_k. Only when the number of these integrals is much smaller than the dimension D of the Hilbert space does it make sense to call the generalized Gibbs state thermal. Otherwise one needs as many Lagrange multipliers β_k to compute the GGE as one has coefficients c_n to describe the initial state of the system. Taking for example again the $|n\rangle\langle n|$'s as integrals of motion one has from eq. 2.2.54 that

$$\frac{\exp\left(-\beta_n I_n\right)}{Z_{GGE}[\{I_k\}](\{\beta_k\})} = |c_n|^2, \tag{2.5.1}$$

where $I_n = |n\rangle\langle n|$. This clearly contradicts the idea of what a thermal state should be. Using our definition of integrability and the corresponding generalized Gibbs ensemble it is possible to define a version of the eigenstate thermalization hypothesis for integrable models where the thermal state corresponds to the GGE ([54], [55]).

2.5.3 Level spacing distributions

We have discussed in the previous section how our notion of integrability leads to differences in the thermalization properties between integrable and non-integrable systems. These thermalization properties can then be been seen as fundamental criteria in the above sense which can used to distinguish the two classes of systems according to their physical behaviours. We are now going to discuss another such property which has proven very popular and which also brings out the connections to the integrability of classical systems. It is the so called *level spacing distribution*. For this we define the set $\{s_i\}$ of nearest

neighbour energy level spacings by

$$s_i := E_{i+1} - E_i \tag{2.5.2}$$

where E_i are the energy values of the system. The probability $p(s)ds$ of s to be a level spacing is defined as

$$p(s)ds := \frac{\text{number of level spacings of value } s}{\text{total number of level spacings}}. \tag{2.5.3}$$

Unfolding of spectra:

In order to be able to compare level spacings of between two local spectral regions with different average level densities (or between different systems) in a meaningful way, it is necessary to locally rescale the unit of energy to obtain a uniform mean spacing throughout the whole spectrum. This is the procedure of *spectral unfolding* [57]. For this it is first necessary to obtain an average density of states defined as

$$G(E) := \frac{1}{D}\sum_{i=1}^{D}\delta(E - E_i), \tag{2.5.4}$$

which is the derivative of the level staircase function

$$N(E) := \frac{1}{D}\sum_{i=1}^{D}\Theta(E - E_i), \tag{2.5.5}$$

counting the number of energy states up to a certain energy. The average density of states is obtained by

$$\overline{G}(E) := \frac{1}{D}\frac{\Delta N}{\Delta E}. \tag{2.5.6}$$

The energy interval ΔE which must be small enough such that only local but no systematic (global) fluctuations appear. On the other hand ΔE must be large enough to contain many energy levels ΔN such that local energy fluctuation do not prevent $\overline{G}(E)$ from being a smooth function of E. One method to practically implement the averaging of the level density [57] is to consider the function

$$G_\Delta(E) := \frac{1}{D}\sum_{i=1}^{D} g(E - E_i). \tag{2.5.7}$$

It is the convolution of $G(E)$ with the Gaussian function

$$g(E) := \frac{1}{\Delta\sqrt{\pi}}\exp(-E^2/\Delta^2). \tag{2.5.8}$$

One then looks for the optimal value of Δ by minimizing the mean square deviation between the level staircase and the integral of $G_\Delta(E)$,

$$N_\Delta(E) := \int_{-\infty}^{E} dE' G_\Delta(E'), \tag{2.5.9}$$

which can be seen as the smooth average level staircase $\overline{N}(E)$.
The unfolding of the spectrum now leads to the task of finding a function $f(E)$ such that the rescaled energy levels, given by

$$e_i = f(E_i), \tag{2.5.10}$$

have globally constant mean spacings which are set to unity. The mean is being evaluated with respect to energy intervals $E - \Delta E/2, E + \Delta E/2$. The function $f(E)$ can be obtained as follows [57]:

$$\begin{aligned} 1 &= \frac{\Delta e}{\Delta N} \\ &= \frac{1}{\Delta N}[f(E + \Delta E/2) - f(E - \Delta E/2)] \\ &= \frac{\Delta E}{\Delta N} f'(E) = f'(E)/\overline{G}(E)D. \end{aligned} \tag{2.5.11}$$

Integration leads to

$$f(E) = D \int_{-\infty}^{E} dE' \overline{G}(E') = D\overline{N}(E). \tag{2.5.12}$$

This means that the rescaled energy level are now given by

$$e_i = D\overline{N}(E_i). \tag{2.5.13}$$

Poisson distribution for integrable models:

Numerical studies ([60], [61], [62]) of integrable models have often shown a distribution of level spacings which is of *Poisson* type. One then speaks of level clustering, because of the tendency of the energy levels to come very close together. Based on semiclassical torus quantization, *Berry* and *Tabor* [59] have been able to derive the Poisson distribution for system whose classical counterparts are integrable in the classical sense. However many of the above mentioned numerics were performed on systems which do not possess any clearly defined classical limit. It is possible to give a derivation of the Poisson probability which is only based on the assumption that the levels form a random sequence without any correlation between them [57]. This can be formalized ([57], [58]) by considering the *spectral autocorrelation function*

$$\begin{aligned} C(E) :&= \langle \rho(\overline{E})\rho(\overline{E} + E)\rangle - \langle \rho(\overline{E})\rangle\langle \rho(\overline{E} + E)\rangle \\ &= \langle \rho(\overline{E})\rho(\overline{E} + E)\rangle - 1, \end{aligned} \tag{2.5.14}$$

where the brackets indicate local averaging over $\overline{E}$ (recall that the local average of $\rho(E) = 1$). In the case of random matrices an ensemble average of the

expression in the brackets has to be performed first. No correlation between eigenvalues then corresponds to

$$C(E) = \delta(E). \tag{2.5.15}$$

Assuming an already unfolded spectrum one considers the conditional probability $g(s)ds$ of finding a level in the interval $[E, E+s]$ if there is one at E. The assumption of no correlations means that $g(s)$ must be a constant as a function of E and s. Denoting by $\Pr(E_1 \cup E_2)dE_1dE_2$ the probability of finding an energy eigenvalue in dE_1 at E_1 and another eigenvalue in dE_2 at E_2, one has

$$\begin{aligned} g(s) :&= \frac{\langle \Pr(E \cup E+s) \rangle}{\langle \Pr(E) \rangle} \\ &= \frac{\langle \rho(E)\rho(E+s) \rangle - \delta(s)}{\langle \rho(E) \rangle} \\ &= C(s) + 1 - \delta(s) \\ &= \delta(s) + 1 - \delta(s) = 1. \end{aligned} \tag{2.5.16}$$

We see that the assumption of no correlations leads to $g(s) = 1$. The probability $p(s)ds$ of finding in ds at $E+s$ the nearest neighbour of the energy level at E can now be written as the product of $g(s)$ times that probability that there is no other level between E and $E+s$,

$$p(s) = g(s) \int_s^\infty ds' p(s'). \tag{2.5.17}$$

Differentiating this equation with respect to s gives

$$\frac{\partial p}{\partial s} = \frac{\partial g}{\partial s} \int_s^\infty ds' p(s') - gp = (g^{-1}\frac{\partial g}{\partial s} - g)p. \tag{2.5.18}$$

The general solution of this equation is

$$p(s) = \text{const}\, g(s) \exp(-\int_0^s ds' g(s')). \tag{2.5.19}$$

Since $g(s)$ must be a constant, by normalizing and scaling such that the global mean spacing

$$\overline{s} := \int_0^\infty ds\, s\, p(s) = 1, \tag{2.5.20}$$

it follows that

$$p(s) = \exp(-s). \tag{2.5.21}$$

This is the Poisson distribution.

Wigner-Dyson distribution:

For systems far away from integrability, and which do not exhibit many body localisation of their energy eigenstates, numerical results ([60], [61], [62]) show that the level spacing distribution is of the *Wigner-Dyson* type. This distribution can also be derived for the *Gaussian ensembles of random matrices* ([66], [67]). These two results indicate that the Wigner-Dyson distribution can be considered as typical in the sense of the discussion in section 2.4.3.
The ensembles are defined by specifying for every Hamiltonian H a probability density $p(H)$ such that

$$\begin{aligned} &\text{(i)} \int p(H_{11}, H_{12}, ..., H_{DD}) dH_{11} dH_{12} ... dH_{DD} = 1, \\ &\text{(ii)}\, p(H) = p(H'),\ H' = OHO^\dagger,\ O^\dagger = O^{-1}, \\ &\text{(iii)}\, p(H_{11}, H_{12}, ..., H_{DD}) = p(H_{11}) p(H_{12}) ... p(H_{DD}) \end{aligned} \tag{2.5.22}$$

Condition number (iii) means that the matrix elements are uncorrelated. For the transformation matrices (the canonical transformations) in condition (ii) one distinguishes between three different types of systems, depending on the transformation properties under the anti unitary time reversal operator $\mathcal{T}$ ([57],[58]). First case one considers systems of spinless particles with time reversal symmetry ($[H, \mathcal{T}] = 0$). In this case $\mathcal{T}$ corresponds to the complex conjugation operator $\mathcal{K}$ (where the complex conjugation is defined with respect to the position basis) with the property that $\mathcal{T}^2 = 1$. The Hamiltonian H can be chosen as a real matrix and the transformation matrices O are orthogonal matrices with $O^\dagger = O^T$. This is the so called Gaussian orthogonal ensemble.
For a system of N spin-1/2 particles $\mathcal{T} = \exp(iS_y/\hbar)\mathcal{K}$, where S_y is the y-component of the total spin operator $S = \hbar(\sigma_1 + \sigma_2 + ... + \sigma_N)/2$. The square of $\mathcal{T}$ now fulfils

$$\mathcal{T}^2 = \begin{cases} +1 & N \text{ even} \\ -1 & N \text{ odd.} \end{cases} \tag{2.5.23}$$

A consequence of $\mathcal{T}^2 = -1$ is *Kramers' degeneracy*, the fact that

$$\langle \Psi | \mathcal{T} \Psi \rangle = 0. \tag{2.5.24}$$

For spin-1/2 systems with time reversal symmetry the matrix elements of the Hamiltonian H can then be combined into 2×2 matrices

$$H_{nm} = \begin{pmatrix} \langle \overline{\Phi}_n | H | \overline{\Phi}_m \rangle & \langle \overline{\Phi}_n | H | \Phi_m \rangle \\ \langle \Phi_n | H | \overline{\Phi}_m \rangle & \langle \Phi_n | H | \Phi_m \rangle \end{pmatrix}, \tag{2.5.25}$$

where $\overline{\Phi}_n = \mathcal{T}\Phi_n$. Using the anti-Hermitian matrices $\tau = -\mathrm{i}\sigma$, the matrix elements of the Hamiltonian can be written as

$$H_{nm} = H_{nm}^{(0)} 1 + \sum_{\mu=1}^{3} H_{nm}^{(\mu)} \tau^{(\mu)}, \tag{2.5.26}$$

where the real coefficients $H_{nm}^{(0)}$, $H_{nm}^{(\mu)}$ characterize the block H_{nm}. They satisfy the relations ([57])

$$\begin{aligned} H_{mn}^{(0)} &= H_{nm}^{(0)} \\ H_{mn}^{(\mu)} &= -H_{nm}^{(\mu)}, \quad \mu = 1, 2, 3. \end{aligned} \tag{2.5.27}$$

This form of the Hamiltonian is referred to as *quaternionic real*. The time reversal operator $\mathcal{T}$ can be written as

$$\mathcal{T} = \mathcal{Z}\mathcal{K}, \tag{2.5.28}$$

where the unitary matrix $\mathcal{Z}$, viewed as a $D \times D$ matrix, is given by

$$\mathcal{Z}_{nm} = \delta_{nm}\tau^{(y)}. \tag{2.5.29}$$

It is now possible to find the unitary transformation matrices S which preserve the form of the the basis spanned by Φ_n, $\overline{\Phi}_n$ and which transform a quaternionic real Hamiltonian into another quaternionic real Hamiltonian [57]. They must satisfy the condition that

$$\mathcal{T} = S\mathcal{T}S^{-1} = S\mathcal{Z}\mathcal{K}S^{-1} = S\mathcal{Z}S^T\mathcal{K}. \tag{2.5.30}$$

From this it follows that

$$S\mathcal{Z}S^T = \mathcal{Z}. \tag{2.5.31}$$

Matrices satisfying this condition are the so called *symplectic matrices*. Using them as the transformation matrices in the above condition (ii) leads to the *Gaussian Symplectic Ensemble* (GSE) for spin- 1/2 particles with time reversal symmetry.

In the general case of no $\mathcal{T}$- invariance the transformation matrices are general unitaries, transforming a Hermitian operator into another, with the property that $U^\dagger = U^{-1}$. The corresponding ensemble is the *Gaussian Unitary Ensemble* (GUE).

By appropriately choosing the zero of energy the following form for $p(H)$ can be derived for all three of the above ensembles ([57],[58])

$$p(H) = C\exp(-A\mathrm{Tr}\{H^2\}), \tag{2.5.32}$$

where A fixes the unit of energy and C is determined by normalization. For the computation of the level spacing distribution (and for comparison with experiments) it is necessary to switch to an eigenenergy representation $p(E_1, ..., E_D)$ of the probability density. From eq. 2.5.32 one obtains ([57],[58])

$$p(E_1, ..., E_D) = \text{const} \prod_{\mu<\nu}^{1...D} |E_\mu - E_\nu|^{n-1} \exp(-A\sum_{\mu=1}^{D} E_\mu^2), \tag{2.5.33}$$

where $n = 2$, 3 or 5 for the GOE, GUE and the GSE respectively. For $D = 2$, eq. 2.5.33 can be used to derive the level spacing distribution $p(s)$, namely

$$\begin{aligned} p(s) =& \text{const} \int_{-\infty}^{+\infty} dE_2 \int_{-\infty}^{+\infty} dE_1 \delta(s - |E_2 - E_1|) \\ & \times |E_2 - E_1|^{n-1} \exp\{-A(E_2^2 - E_1^2)\} \end{aligned} \tag{2.5.34}$$

where E_1, E_2 are the two eigenvalues of H. Choosing A in such a way that the mean spacing is unity, $\int dss p(s) = 1$, and normalizing such that $\int ds p(s) = 1$, yields

$$p(s) = \begin{cases} (s\pi/2)\exp(-s^2\pi/4) & \text{GOE} \\ (s^2 32/\pi^2)\exp(-s^2 4/\pi) & \text{GUE} \\ (s^4 2^{18}/3^6\pi^3)\exp(-s^2 64/9\pi) & \text{GSE.} \end{cases} \tag{2.5.35}$$

These are the so called Wigner surmises. For general values of D the results differ from the Wigner-Dyson distribution. However, in the especially interesting limit $D \to \infty$ the Wigner surmises are approached ([57],[58]), provided the local mean density is uniform (after the proper spectral unfolding has been performed).

Finally it is important to stress that for systems with symmetries level spacing statistics are only meaningful in a certain symmetry sector. If different symmetry sectors are mixed, level repulsion (Wigner-Dyson statistics) may be missed even for systems far from integrability ([61], [68], [69]).

2.5.4 Delocalization measures

Shannon enropy:

For an eigenstate $|\psi_n\rangle$ of the Hamiltonian H the Shannon (information) entropy S_n with respect to the basis $|\phi_k\rangle$ $(k = 1, ..., D)$ is defined as

$$S_n := -\sum_{k=1}^{D} |c_n^k|^2 ln |c_n^k|^2, \tag{2.5.36}$$

where $|\psi_n\rangle = \sum_{k=1}^{D} c_n^k |\phi_k\rangle$. It measures the number of basis vectors $|\phi_k\rangle$ that contribute to the state $|\psi_n\rangle$. For integrable models as well as for many body localised systems, for which the energy eigenstates can be be considered as localised in some basis, S_n shows strong fluctuations throughout the whole spectrum [rigol].
For random matrices the coefficients c_n^k can be considered as independent random numbers and all energy eigenstates are completely delocalized in any basis. For the GOE one obtains for the average value over the ensemble [61]

$$S_{\text{GOE}} = \ln(0.48D) + \mathcal{O}(1/D), \tag{2.5.37}$$

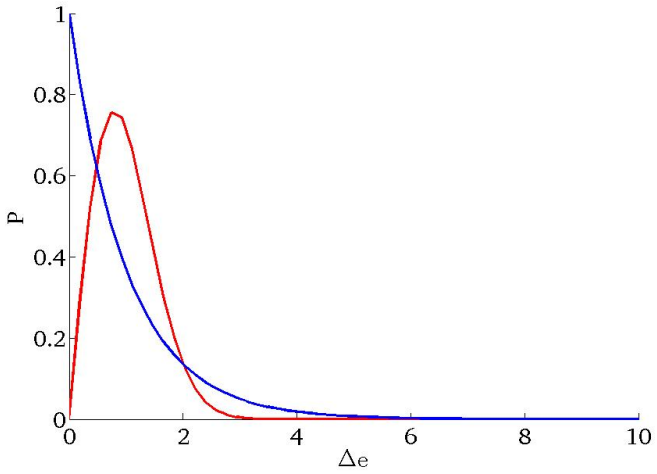


Figure 2.1: Normalized Poisson distribution (blue curve) and Wigner-Dyson distribution (red curve) for nearest neighbour level spacings plotted against the energy differences Δe of the unfolded levels. The main difference, as explained in the main text , is the level clustering in the Poisson distribution and Level repulsion for Wigner-Dyson statistics.

which is however different from the maximum value $S = \ln D$. The GOE-value is also expected for systems far from integrability and for eigenstates around the center of the spectrum.

Inverse participation ratio (IPR):

In analogy with the Shannon entropy the inverse participation ratio IPR_n with respect to the basis $|\phi_k\rangle$ $(k = 1, ..., D)$ is defined as

$$\mathrm{IPR}_n := \frac{1}{\sum_{k=1}^{D} |c_n^k|^4}, \tag{2.5.38}$$

and can equally be viewed as a measure of the number of basis states $|\phi_k\rangle$ which significantly contribute to $|\psi_n\rangle$. It is analogous to the notion of the effective dimension in section 2.3.3. The statements made about the Shannon entropy with respect to the transition from integrability to quantum chaos all apply equally to the IPR.

3 Results

3.1 The systems and observables considered

Our model consists of $N = 5$ spinless fermions on a 19-site, two-dimensional lattice (figure 3.1). The Hamiltonian H is given by

$$\widehat{H} = -t \sum_{\langle i,j \rangle} (\widehat{c}_i^\dagger \widehat{c}_j + h.c.) + V \sum_{\langle i,j \rangle} \widehat{n}_i \widehat{n}_j \tag{3.1.1}$$

where $\langle i, j \rangle$ indicates that the sum is taken over nearest-neighbour sites, t is the hopping parameter, V the nearest-neighbour repulsion and $\widehat{n}_i = \widehat{c}_i^\dagger \widehat{c}_i$ is the density operator. The units have been chosen in such a way that $\hbar = 1$. Our work was strongly inspired by [5], where the authors study 5 spinless hardcore bosons on a lattice of 21 sites. Our lattice differs from their lattice by removing two sites.

The main difference between the two systems is that fermionic creation ($\widehat{c}_i^\dagger$) and annihilation ($\widehat{c}_j$) operators satisfy the anti-commutation relations

$$\{\widehat{c}_j, \widehat{c}_i^\dagger\} = \{\widehat{c}_j, \widehat{c}_i\} = \{\widehat{c}_j^\dagger, \widehat{c}_i^\dagger\} = 0 \tag{3.1.2}$$

for all i and $i \neq j$ and

$$\{\widehat{c}_i, \widehat{c}_i^\dagger\} = 1 \tag{3.1.3}$$

for all i, where $\{A, B\} := AB + BA$ is the anti-commutator of the operators A and B. When $V = 0$, we have a system of free fermions which is integrable. A single-particle canonical transformation of the creation and annihilation operators diagonalizes the Hamiltonian, and the occupation numbers of these new modes are the integrals of motion.
Hardcore-boson creation ($\widehat{b}_i^\dagger$) and annihilation ($\widehat{b}_j$) operators on the other hand commute on different sites,

$$[\widehat{b}_j, \widehat{b}_i^\dagger] = [\widehat{b}_j, \widehat{b}_i] = [\widehat{b}_j^\dagger, \widehat{b}_i^\dagger] = 0 \tag{3.1.4}$$

for all i and $i \neq j$, where $[A, B] := AB - BA$ is the commutator of the operators A and B. The hardcore condition imposes the anti-commutation relations

$$\{\widehat{b}_i, \widehat{b}_i^\dagger\} = 1, \tag{3.1.5}$$

and

$$(\widehat{b}_i^\dagger)^2 = (\widehat{b}_i)^2 = 0 \tag{3.1.6}$$

for all i. This implies that each site can be occupied by at most one particle, as is the case for fermions. However in contrast to fermions, even when $V = 0$, the system of hardcore-bosons is not integrable, because the hardcore condition ensures that it cannot be diagonalized by a single-particle canonical transformation of the creation and annihilation operators.

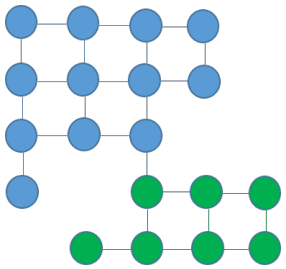


Figure 3.1: The 19-site lattice of the model system studied in this work, which consists of 5 spinless fermions with Hamiltonian defined in eq. 2.1.1. In comparison with the lattice of the system used in [5], 2 additional sites have been removed. The 7 green sites in the lower part represent the subsystem whose ground state serves as the initial state for the time evolution of $n(k_x = 0)$ shown in figure 3.2.

In order to study the dynamics of our fermionic system we have performed a full diagonalization of H (dimension $D = 11628$), which was achieved to machine precision. The observable we studied was the marginal momentum distribution along the horizontal axis, $n(k_x) := \sum_{k_y} n(k_x, k_y)$, where

$$n(k_x, k_y) := 1/L^2 \sum_{i,j} e^{-i2\pi \mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)/L} \langle \hat{c}_i^\dagger \hat{c}_j \rangle. \tag{3.1.7}$$

Here $L := L_x = L_y = 5$ are the linear sizes of the lattice and $\mathbf{r}_i = (i_x d, i_y d)$, where d is the lattice constant. For the summation over k_y in $n(k_x)$ we have divided the first Brillouin zone $[-\frac{\pi}{d}, \frac{\pi}{d}]$ of the k_y-axis into 15 points, uniformly distributed around 0. The summation is done over these points (in comparison [6] have summed over 50 uniformly distributed points).
This quantity is not a mascroscopic obervable in the sense described in section 4.2. However according to the generalization of Von Neumann's typicality approach in [46] fulfilment of the eigenstate thermalization hypothesis is to be expected.

We are looking at the system for different values of V to see how the properties change as we move from the integrable to the non integrable case.

3.2 Time evolution

We want to first look at the time evolution of $n(k_x)$ and see whether we can observe relaxation and thermalization. For this we choose as our initial state $|\psi(0)\rangle$ (analogous to [5]) the ground state of the 5 fermions when they are confined to the 7 sites in the lower part of the lattice (see figure 3.1). We then let them expand over the whole lattice by opening the link, as indicated in the figure. The fact that there is only one link to the upper part ensures that the energy width of the initial state in the eigenstate basis (of the large system on the full lattice) is small ([5], see supplementary information). It is important

to note that this state does not classify as a typical initial sate in cold atom experiments as described in section 2.2.4.

Denoting the eigenstates of H by $|\alpha\rangle$, the initial state can be expanded as

$$|\psi(0)\rangle = \sum_{\alpha} C_{\alpha}|\alpha\rangle, \tag{3.2.1}$$

where $C_{\alpha} = \langle\alpha|\psi(0)\rangle$. For the time evolution of $n(k_x)$ one then gets

$$\langle n(k_x)(t)\rangle = \sum_{\alpha,\beta} C^*_{\alpha} C_{\beta} \exp^{i(E_{\alpha}-E_{\beta})t} \langle\alpha|n(k_x)|\beta\rangle, \tag{3.2.2}$$

where E_{α} are the eigenenergies of $|\alpha\rangle$. In figure 3.2 we compare the time evolution of $n(k_x)$ for $k_x = 0$ to the infinite time averaged value and the microcanonical average. This is done for different values of the interaction strength V. The infinite time averaged state corresponds in the case of no degeneracies (for all $V \neq 0$) to the diagonal ensemble $\rho_{\text{diag}} = \sum_{\alpha} |C_{\alpha}|^2 |\alpha\rangle\langle\alpha|$ (see 2.3.1), so one has

$$\langle n(k_x)(t)\rangle_{\infty} = \langle n(k_x)\rangle_{\rho_{\text{diag}}} = \sum_{\alpha} |C_{\alpha}|^2 \langle\alpha|n(k_x)|\alpha\rangle. \tag{3.2.3}$$

For the microcanonical ensemble we are averaging over all eigenstates of H that lie within a narrow window $[E_0 - \Delta, E_0 + \Delta]$, where $E_0 = \langle\psi(0)|H|\psi(0)\rangle$ is the mean energy in the initial state and $\Delta = 0.1t$.

One can now try to use Theorem 1 from 2.3.1 to infer whether equilibration takes place in the infinite time limit. By taking the limits $T \to \infty$ and $\varepsilon \to 0$ in inequality 2.3.21 one obtains

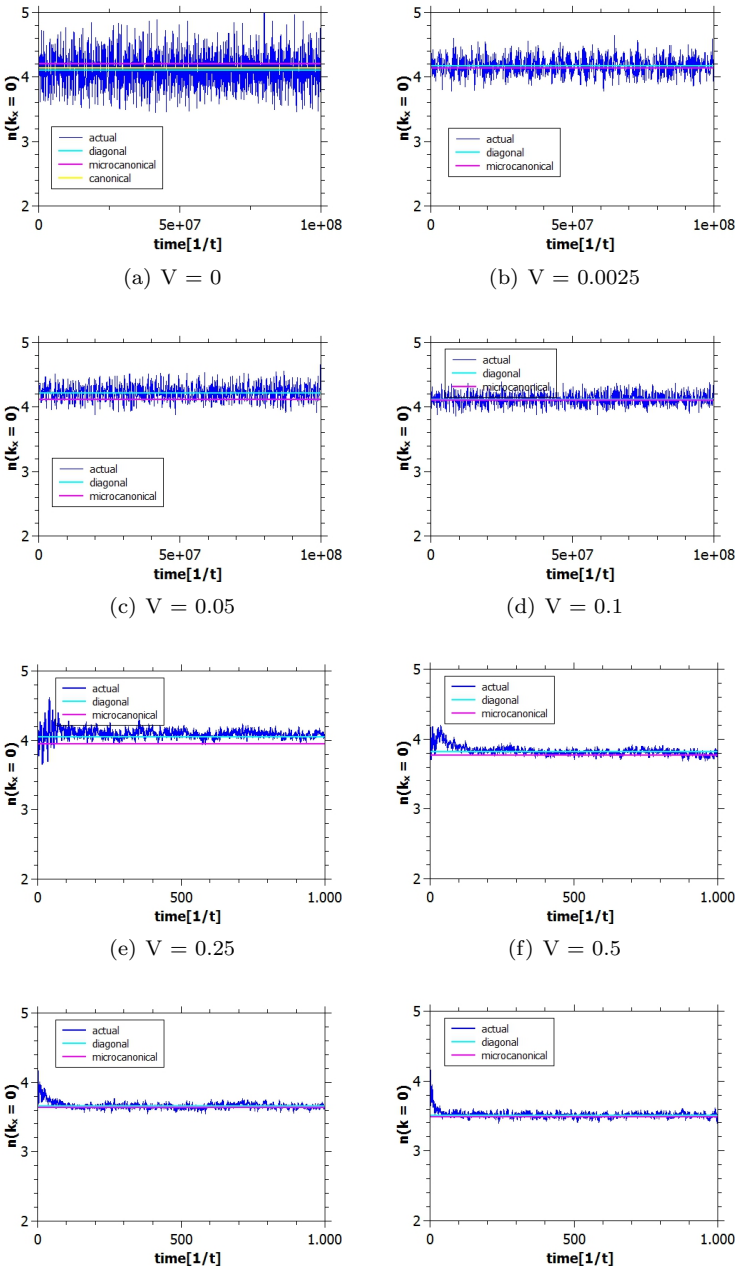
$$\sigma^2_{n(k_x=0)}(T \to \infty) \leq ||n(k_x = 0)||^2_{\infty} N(0) g((p_{E_n})_1^{d'}). \tag{3.2.4}$$

As explained in 2.2.4 and 2.3.1, one can only speak of equilibration when $\sigma_A(T \to \infty) \leq \delta A$. Since it is nowadays possible in cold atom experiments [Bloch] to measure $n(k_x)$ to within $1 - 2\%$ precision, one has to take these values for $\delta n(k_x = 0)$. Due to the small size of our systems, for no value of V which we have used in our computations the left hand side of 3.2.4 is small enough for the above condition to be fulfilled. The number of occupied energy eigenstates in the diagonal ensemble (see Theorem 1), although growing with increasing V, is simply too small. As a result the quantity $g((p_{E_n})_1^{d'})$ is too large and we cannot use Theorem 1 to infer infinite time equilibration in our models. In figure 3.5 we plot $g((p_{E_n})_1^{d'})$ against the interaction strength V.
Additionally for the non interacting integrable model at $V = 0$ the degenerate energy gaps condition (see section 2.3.3) is strongly violated (it is fulfilled for the all the other systems considered). Additonally to the integrablilty there is a 3-fold degeneracy in the spectrum of the corresponding single particle Hamiltonian (see 3.5.1). As a result the maximum number of degenerate gaps $N(0)$ in eq 3.2.4 is much larger than 1. This apparently explains the large fluctuations

in figure 3.2 a).
However, figure 3.2 indicates that for the 3 largest values of V equilibration is achieved or at least almost achieved during the finite time intervals considered.

In figure 3.3 we are testing the equilibration condition imposed by the second part of the ETH (see section 2.4, we note that the non-degenerate gaps condition is valid for all the systems with $V \neq 0$ we have considered). For this we plot the absolute values of the matrix elements of $n(k_x)$ in the energy eigenbasis for certain consecutive eigenstates around E_0. It is clear that we cannot test in this numerical simulation the full condition which states that the off diagonal matrix elements are exponentially small in the system size. Our aim here is to show that at least they are much smaller than the diagonal matrix elements [5]. Again we compare the results for the different values of V. One can see that the condition is well fulfilled for all value of V considerd by us, although for the smaller V's the fluctuations of the off diagonal elements, although still smaller than the diagonal ones, increase.

Finally in figure 3.4 we compare the equilibration times $T_{\min}$ of the 3 systems with largest values of V with the 2 minimal time scales $t_{\min}$ and $T_{\min}$ introduced in section 2.3.4 (we have set here $T_{\min} = \frac{d'}{\Delta E}$. As one can see in all 3 cases $T_{\min}$ is much closer to $t_{\min}$ (but larger as it must be). This is to be expected because of the very general nature of theorem 1, from which $T_{\min}$ has been derived (see section 2.3.4).



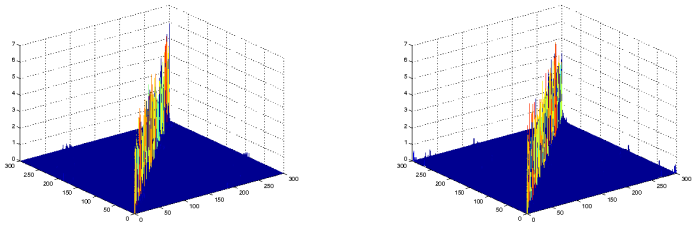
(a) V = 0 (b) V = 0.0025

(c) V = 0.05 (d) V = 0.1

(e) V = 0.25 (f) V = 0.5

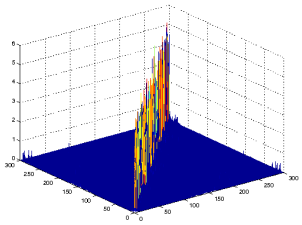
(g) V = 0.75 (h) V = 1

Figure 3.2: Time evolution of $n(k_x = 0)$ for different values of V ((a)-(h)). V is measured in the strength of the hopping parameter t, and time is measured in its inverse. The actual values are compared to the microcanonical and diagonal ensembles. The initial states are as described in the main text.

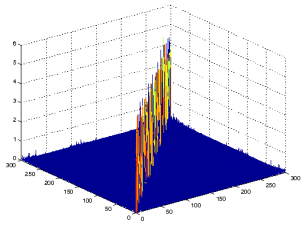


(a) V = 0

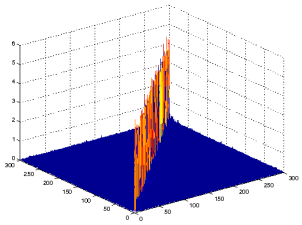
(b) V = 0.0025



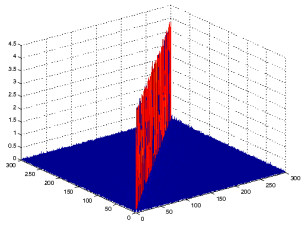
(c) V = 0.05



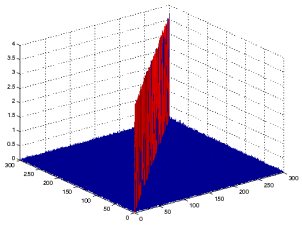
(d) V = 0.1



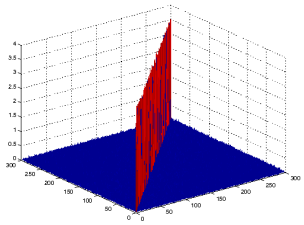
(e) V = 0.25



(f) V = 0.5

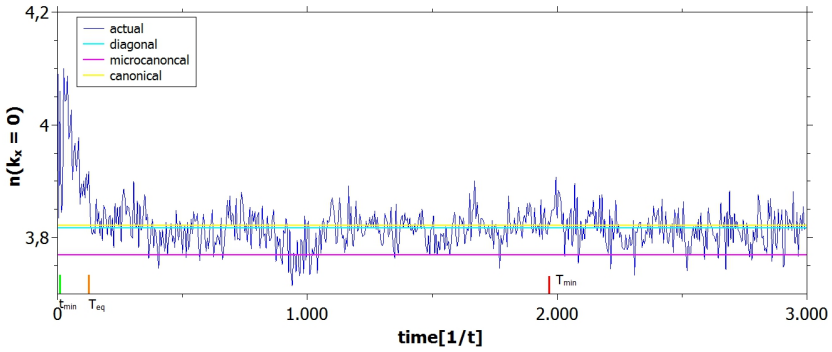


(g) V = 0.75

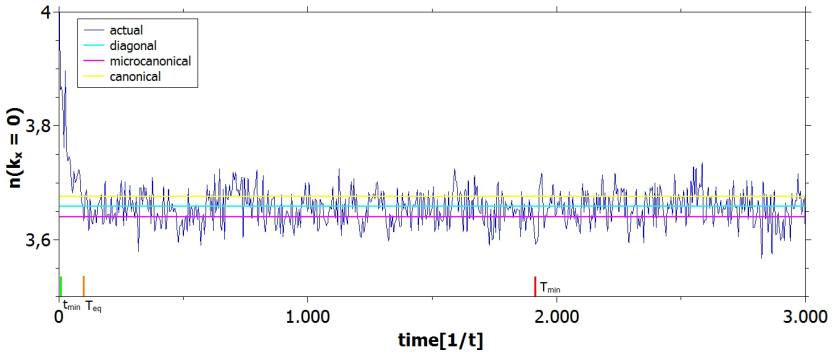


(h) V = 1

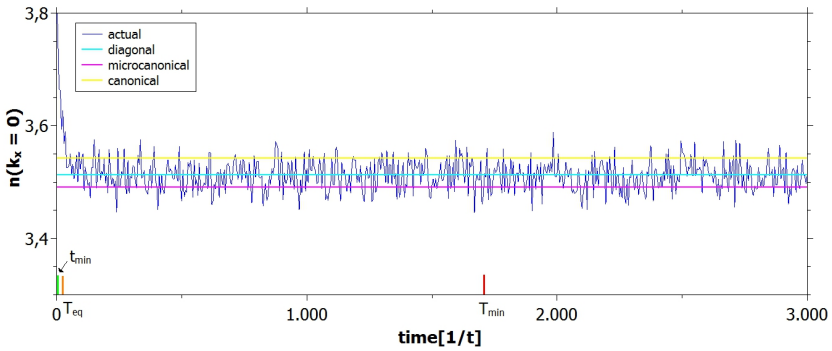
Figure 3.3: The absolute values of the matrix elements of $n(k_x = 0)$ in the energy eigenbasis computed for 300 consecutive eigenstates around E_0. The results are compared for different values of V ((a)-(h)).



(a) V = 0.5



(b) V = 0.75



(c) V = 1

Figure 3.4: For better comparison of the various time scales we again plot the time evolution of $n(k_x = 0)$ for the 3 largest values of V. Indicated in the graphics are the 2 minimal times T_{min} and t_{min}, which are explained in the main text and compared to the equilibration time T_{eq}.

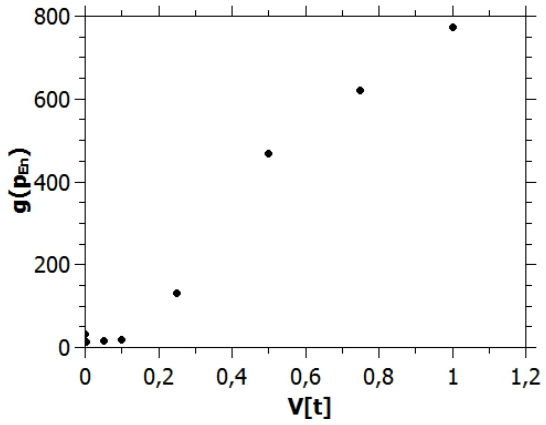


Figure 3.5: The parameter $g(p_{E_n})$, which measures the number of occupied energy eigenstates in the diagonal ensemble, as a function of the interaction strength V

.

3.3 Momentum distribution

We now want to study the values of $n(k_x)$ for different k_x in the diagonal- and microcanonical ensembles. We are again varying the interaction strength V.

In figure 3.6 we compare the 2 ensembles for 25 different values of k_x which have been uniformly distributed on the first Brillouin zone of the k_x-axis. For comparison we also include the values of $n(k_x)$ in the initial states. One can see that as V is increasing the values match better and better. Especially for the largest 3 values of V, for all k_x, the differences between them are getting close to $\delta n(k_x = 0)$ discussed in the previous section. In these cases one can then speak of thermalisation in the sense defined in section **??**. For the smaller values of V there are certain k_x for which the difference between the 2 ensembles is also very small, but in general it is clearly larger.

To answer the question whether the ETH (see section 2.4.2) is responsible for the thermalisation or failed thermalisation of $n(k_x)$ for the particular systems, we computed in figure 3.7 the values of the central component $n(k_x = 0)$ in the eigenstates of the Hamiltonian. In addition we plot the probability p of each eigenstate in the initial state $|\psi(0)\rangle$ to see which eigenstates have the highest weights in the diagonal ensemble (the probabilities are equal to the $|C_\alpha|^2$ for the C_α in eq. 3.2.1). Both quantities are plotted against the particular eigenenergies of the eigenstates. One sees very nicely how $n(k_x = 0)$ changes slowly from a wildly fluctuating behaviour into an almost smooth function of the eigenenergies as V is increasing.

In figure 3.8 we plot the canonical predictions for $n(k_x)$ and compare them

to the diagonal and microcanonical values. The temperature of the canonical ensemble is computed by solving eq. 2.2.37 for β and setting E_{mean} equal to the mean energy of the initial state E_0. As explained in section 2.2.6 the observed differences are a consequence of the finite size of our systems. One observes that in general the microcanonical predictions are slightly closer to the diagonal ones than the canonical predictions.

To strengthen the case for the validity of the ETH for large values of V and its failure for smaller ones, we compute in figure 3.9 $n(k_x)$ for 100 consecutive eigenstates around E_0. We then plot the mean values and variances against k_x. Again one observes how the fluctuations decrease drastically as the interaction strength increases.

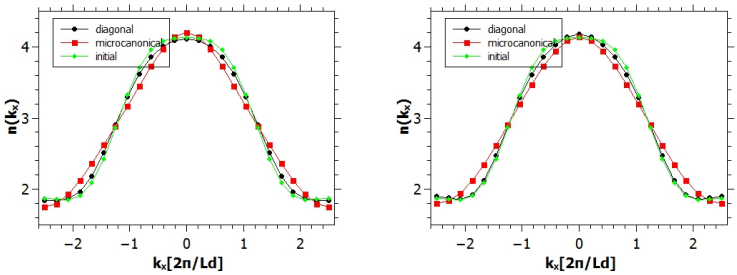
Figures 3.7 and 3.9 strongly indicate that eigenstate thermalistation fails for small values of V but gets fulfilled more and more accurately as V becomes larger. However as already mentioned above, in 3.6 there are individual values of k_x where the the two ensembles are very close, such that thermalisation still happens for these values. To find out what is the reason for the apparent thermalisation we plot in figure 3.10 again the fluctuations of $n(k_x)$ in the energy eigenstates and compare them to the corresponding probabilities of the diagonal ensemble as in figure 3.7. This time however we chose a much smaller number of eigenstates from the vicinity of E_0 used for the microcanonical ensemble. This allows us to investigate which of the 3 conditions of section 2.4.2 is responsible for the thermal behaviour.
For $V = 0$ the ETH is not fulfilled in the cases of $n(k_x = 1.875)$ and $n(k_x = 1.25)$. In figure 3.10 (a) and (b) we see that in both cases there are correlation between the values of the probabilities and the values of $n(k_x)$ in the particular eigenstates. This is to be expected as ETH is not fulfilled in the cases of represents an integrable system.
The ETH is also not fulfilled in the case of $V = 0.1$ for $n(k_x = 0)$. However in that case we observe thermalisation according to figure 3.6 (ignoring for now the dynamical fluctuations during time evolution in figure 3.2). In figure 3.10 (c) one can see that here both the fluctuations of the $n(k_x)$ and the fluctuations of the probabilities are large, which excludes condition 3, the equality of all probabilities. However, the fluctuations are unbiased in that case and so condition 1 is the underlying reason for the small differences between the diagonal and microcanonical predictions.
In contrast we have seen that for $V = 0.25$ the fluctuations of $n(k_x = 0)$ in the corresponding energy eigenstates are much smaller than in the previous two examples, such that the ETH is approximately fulfilled. However figure 3.6 shows that the the microcanonical and diagonal ensemble predictions differ in that case. In figure 3.10 (d) one sees that for the case of $V = 0.25$ there are correlations between the values of $n(k_x = 0)$ and P. For most eigenstates with significant values of P, the $n(k_x = 0)$ are larger than the microcanonical values. As such the microcanonical ensemble gives a smaller value than the prediction from the diagonal ensemble.

For completeness we also show the case of $V = 1$, where the ETH is valid and no apparent correlations between P and $n(k_x = 0)$ can be observed as expected, since the system with $V = 1$ is already far from integrability.

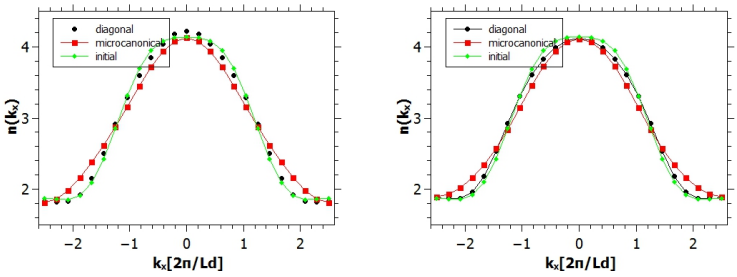
Finally we have to address the dependence of the microcanonical ensemble on the size of the energy width Δ defined in section 3.2. Since we are dealing here with a small system, making Δ too small would mean that at some point here would be no eigenstates left in the energy window around E_0 [5]. All one can do is to test the robustness of the microcanonical predictions with respect to sizes of Δ which are not too small. In figure Δfig:microcanonical distribution with smaller ΔEe compare our original microcanonical ensemble defined for $\Delta = 0.1t$ to a second ensemble defined for $\Delta = 0.05t$. As expected one sees stronger robustness in the cases of larger V.

3.4 Measurement fluctuations

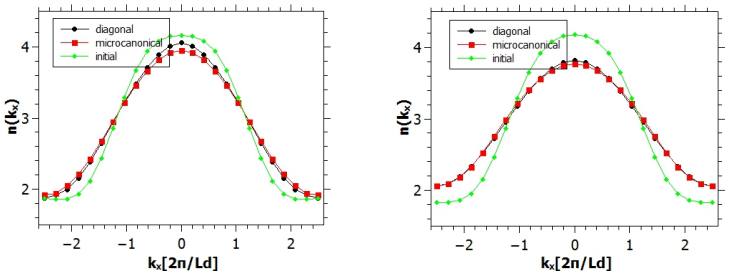
So far we have only considered expectation values. However it is well known that in the usual ensembles of statistical mechanics fluctuations around mean values scale like $1/\sqrt{N}$ (see section 2.2.6). Since we are dealing here with small systems quantum fluctuations in the time dependent states measurement to measurement fluctuations) in figure 3.2 are expected to be large [5]. This is confirmed in figure of 3.12 were we plot the time evolution of $n(k_x = 0)$ together with the variance at each point in time.



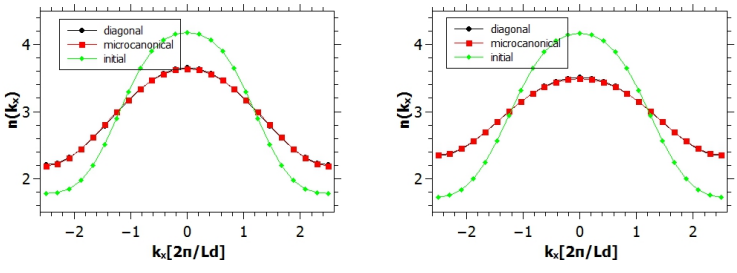
(a) V = 0 (b) V = 0.0025



(c) V = 0.05 (d) V = 0.1

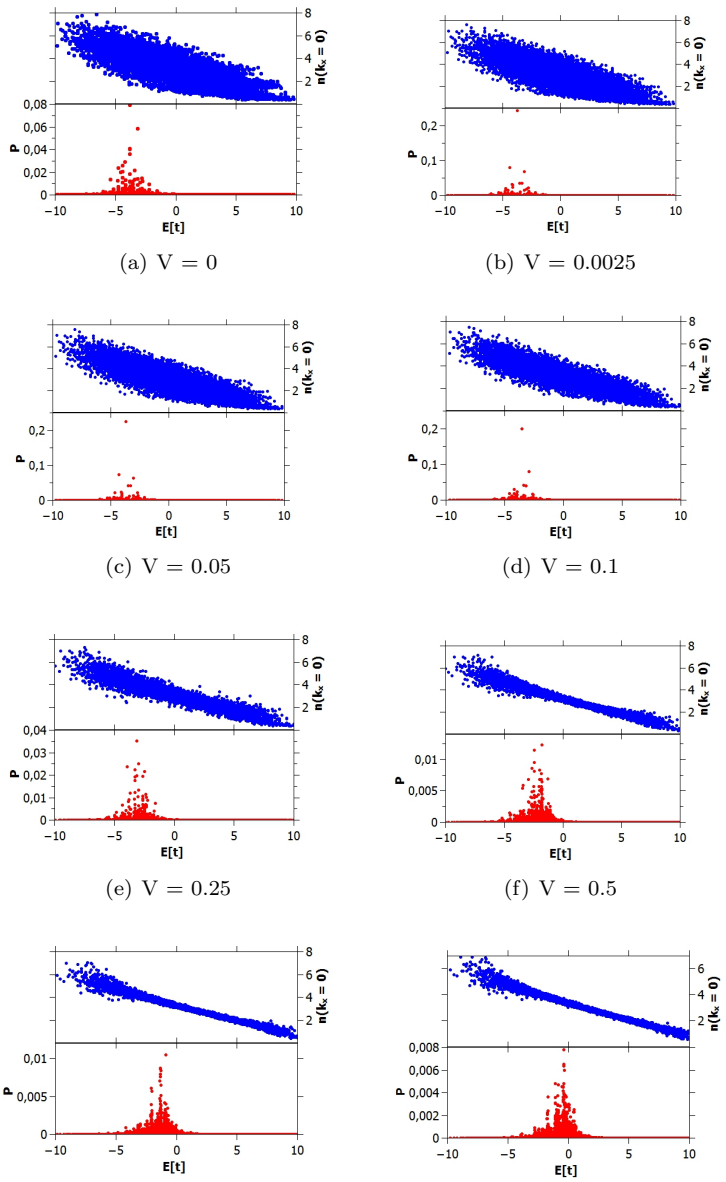


(e) V = 0.25 (f) V = 0.5



(g) V = 0.75 (h) V = 1

Figure 3.6: The values of $n(k_x)$ in the diagonal- and microcaonical ensembles, as well as in the initial state, compared for different values of V ((a)-(h))



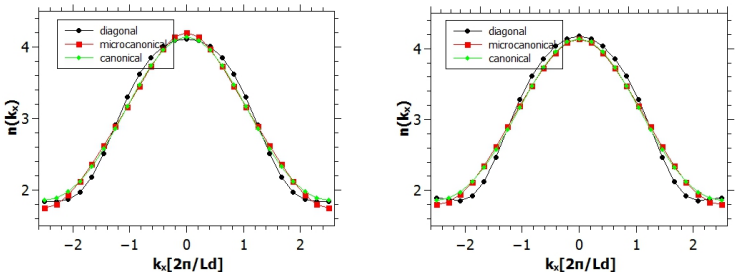
(a) V = 0 (b) V = 0.0025

(c) V = 0.05 (d) V = 0.1

(e) V = 0.25 (f) V = 0.5

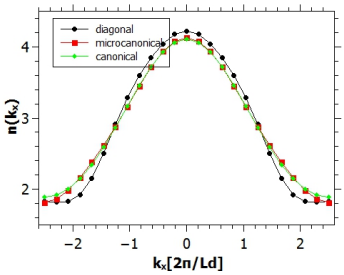
(g) V = 0.75 (h) V = 1

Figure 3.7: $n(k_x = 0)$ and probability p of individual eigenstates in the diagonal ensemble as functions of the eigenstate energy for different values of V ((a)-(h)).

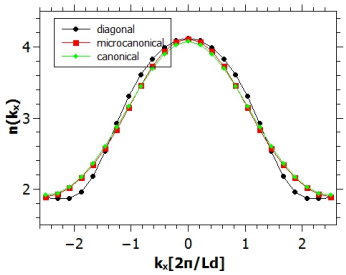


(a) V = 0

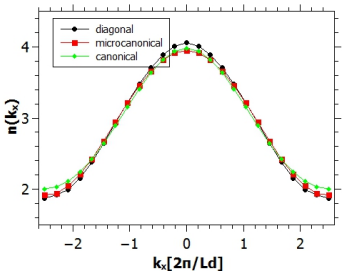
(b) V = 0.0025



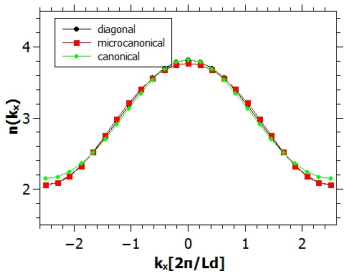
(c) V = 0.05



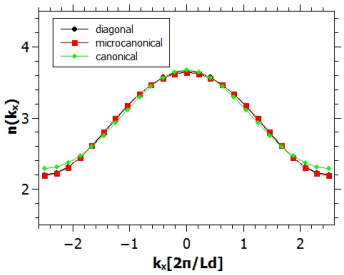
(d) V = 0.1



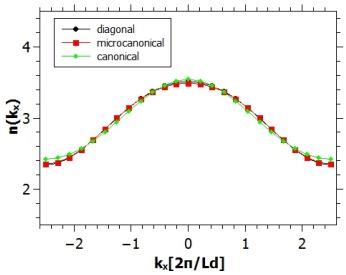
(e) V = 0.25



(f) V = 0.5

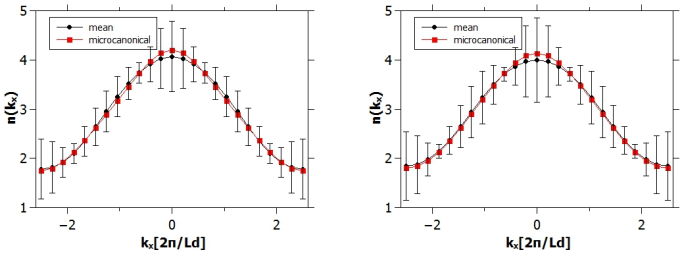


(g) V = 0.75

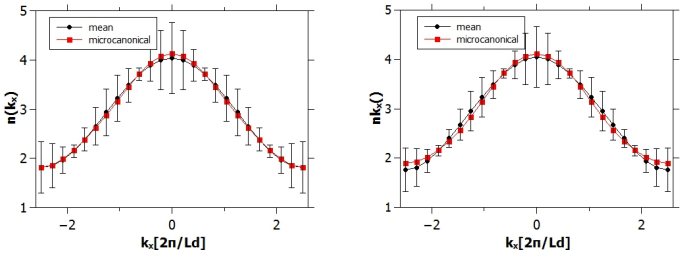


(h) V = 1

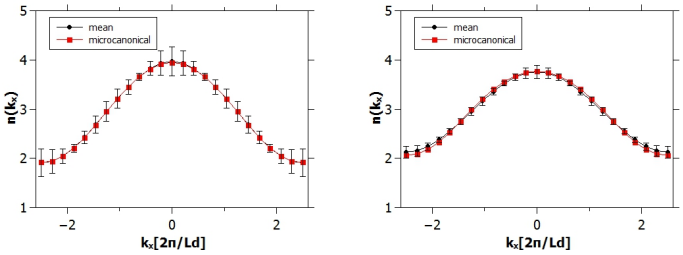
Figure 3.8: The canonical predictions for $n(k_x)$ compared to the diagonal and microcanonical values. As explained in the main text the difference between the canonical and microcanonical ensembles are due to the finite size of the systems considered. The temperature of the canonical ensemble is computed from eq. 2.2.37.



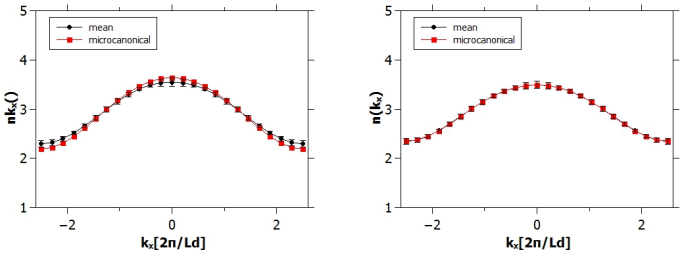
(a) V = 0 (b) V = 0.0025



(c) V = 0.05 (d) V = 0.1

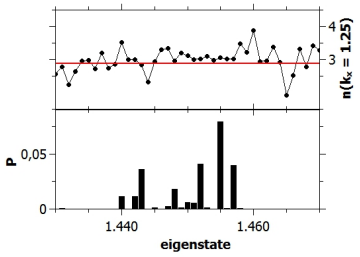


(e) V = 0.25 (f) V = 0.5

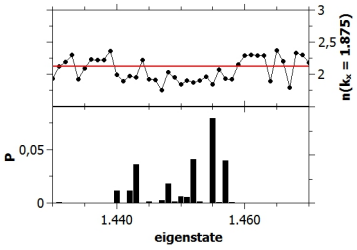


(g) V = 0.75 (h) V = 1

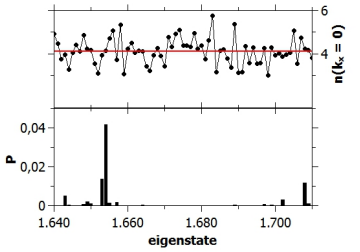
Figure 3.9: The means and variances of $n(k_x)$ for 100 consecutive eigenstates around E_0 compared to the microcanonical values. Again V is varied as above ((a)-(h)).



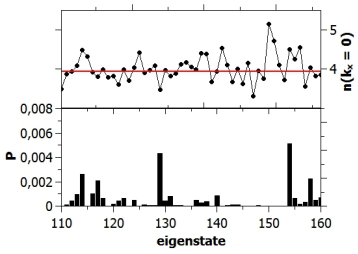
(a) V = 0



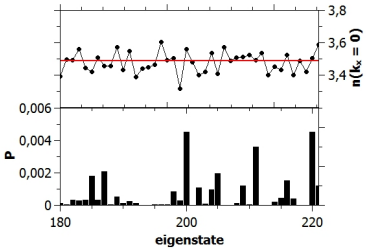
(b) V = 0



(c) V = 0.1

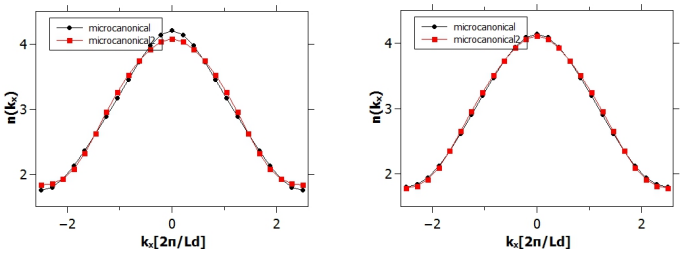


(d) V = 0.25



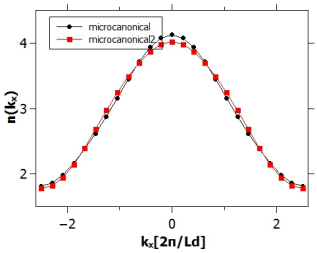
(e) V = 1

Figure 3.10: To test which of the 3 mechanisms introduced in section 2.4.2 is responsible for thermalistation (or failure to thermalize) we plot the values of $n(k_x)$ and the probabilities P for various eigenstates with energy values close to E_0.

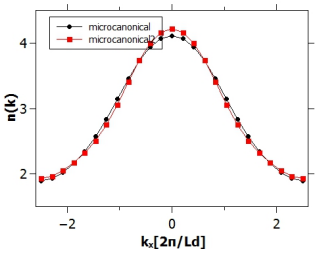


(a) V = 0

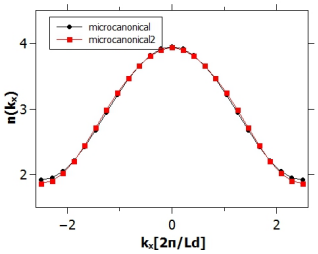
(b) V = 0.0025



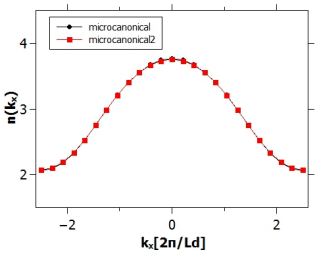
(c) V = 0.05



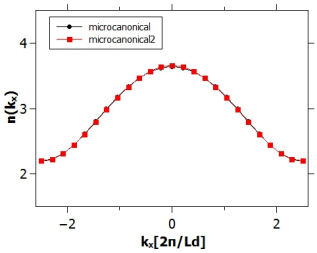
(d) V = 0.1



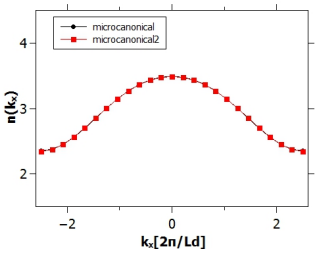
(e) V = 0.25



(f) V = 0.5

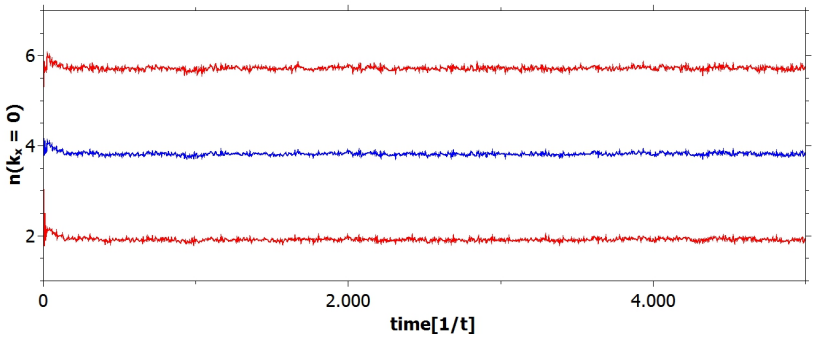


(g) V = 0.75

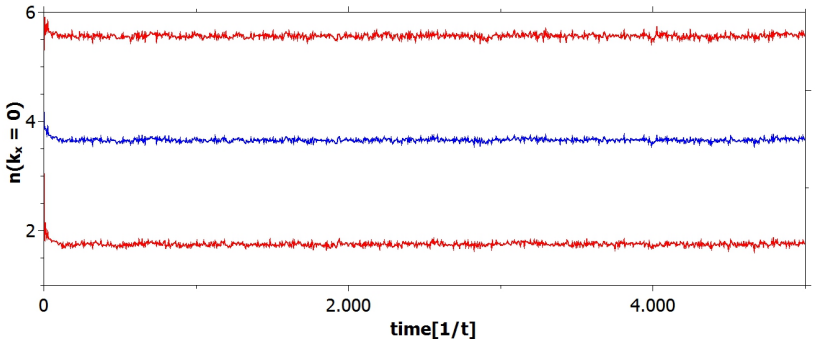


(h) V = 1

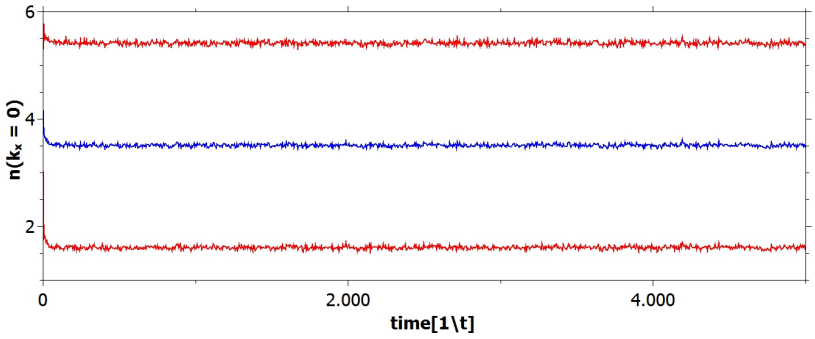
Figure 3.11: Comparison between the original microcanonical prediction for $\Delta = 0.1t$ and a second microcanonical ensemble (microcanonical2 in the figure) with $\Delta = 0.05t$.



(a) V = 0.5



(b) V = 0.75



(c) V = 1

Figure 3.12: We plot again the time evolution of $n(k_x = 0)$ (blue line). This time we add for each time dependent state the variation, represented through the two red lines, of $n(k_x = 0)$ in that state.

3.5 Signatures of the transition to quantum chaos

We have studied the changing of three quantities (with varying V) for the transition from integrability to quantum chaotic (and thermal) behaviour. The first is the distribution of spacing of neighbouring energy levels s, which depends only on the spectrum. The other two are Shannon entropy S and the inverse participation ratio IPR. Both depend on the eigenstates of the integrable Hamiltonian at $V = 0$.

3.5.1 Level spacings

As explained in section 2.5.3, we expect to see a change in the level spacing distribution as we move away from integrability from Poisson to Wigner-Dyson statistics. In figure 3.13 we plot the level spacing distribution for various values of V. In each case we also plot the Poisson- and Wigner-Dyson distribution for comparison.
We have performed the unfolding of the spectrum (as explained in section 3.5.1) by fitting the staircase function $N(E)$ with a polynomial of degree 15 [5] to obtain smooth averaged $\overline{N}(E)$. 20% of the energy levels at the edges of the spectrum, where fluctuations are largest, have been discarded.
As one can see the distribution develops smoothly from a huge peek at $s = 0$ for $V = 0$ to a nearly Poissonian distribution for small V and then to the Wigner-Dyson form for larger V. The why there is a peak instead of the Poisson form (as expected for an integrable system) at $V = 0$ is a 3-fold degeneracy in the center of the spectrum of the corresponding single particle Hamiltonian (one particle hopping on the lattice). As the eigenstates of the 5-particle system are Slater-Determinants of the single particle eigenstates, this explains the huge peak at $s = 0$. The 3 degenerate single particle eigenstates are localised at a sublattice, whereas the other non-degenerate eigenstates are delocalized. This degeneracy cannot be caused by a symmetry since the only possible symmetries would be a point group symmetries and the time reversal symmetry $\mathcal{T}$. However the 19-site lattice does not poses a point group symmetry and the time reversal symmetry fulfils $\mathcal{T}^2 = 1$. Similar peaks peaks have been observed in [44], where they have been linked to a quasi degeneracy due to time reversal symmetry. Turning on the interaction V the degeneracies get split and the peak disappears. For small V's the distribution is nearly Poisson and smoothly changes into Wigner-Dyson upon increasing V. This is the expected transition which has been described in section 2.5.3.

3.5.2 Shannon entropy

If we denote by $|\psi_n\rangle$ the eigenvectors of the Hamiltonian for a certain value of $V \neq 0$ and by $|\phi_k\rangle$ the eigenvectors of the integrable model for $V = 0$, then the Shannon entropy of $|\psi_n\rangle$ with respect to the $|\phi_k\rangle$ as defined in section 2.5.4 is

given by

$$S_n = -\sum_{k=1}^{D} |c_n^k|^2 ln|c_n^k|^2. \tag{3.5.1}$$

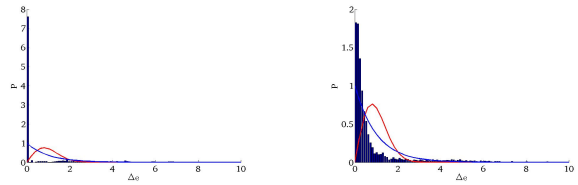
In figure 3.14 we plot S_n against energy for all energy eigenstates and for systems with various values of V. For systems close to the integrable point with small V one observes strong fluctuations of S_n in all regions of the spectrum. As V increases the fluctuations around the center of the spectrum decrease and only remain at the edges of the spectrum. This confirms our expectations that as one moves away from integrability the eigenstates of the Hamiltonian with energies around the center of the spectrum become delocalized in the eigenbasis of the integrable model. This result shows that as expected delocalization of energy eigenstates goes hand in hand with thermal behaviour in the sense of the eigenstate thermalization hypothesis [61].
As was seen in above results (see figures 3.6-3.9) an analogous smooth change in thermalization properties was observed. In particular the fact that even far away from integrability the states at the edges of the spectrum do not show delocalization (as well as violate the ETH) indicates that the Shannon entropy should be regarded as a better indicator of quantum chaos (and thermalization) than level spacing distributions.

3.5.3 Inverse participation ratio

With the same notation as for the Shannon entropy the inverse partitipation ration $\text{IPR}_n of\ |\psi_n\rangle$ with respect to $|\phi_k\rangle$ as defined in section 2.5.4 measures is given by

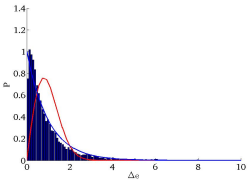
$$\text{IPR}_n := \frac{1}{\sum_{k=1}^{D} |c_n^k|^4}. \tag{3.5.2}$$

In figure 3.15 the IPR_n of all energy eigenstates is plotted against energy for systems with various values of V. As for the Shannon entropy one sees strong fluctuations for small V and smooth behaviour around the center of the spectrum as V increases. This indicates as for S that the IPR should be regarded as a better indicator of quantum chaotic behaviour as well as thermal behaviour than level spacing distributions.

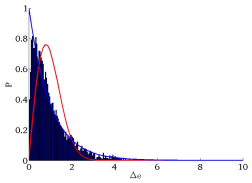


(a) V = 0

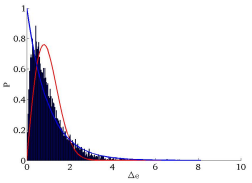
(b) V = 0.0025



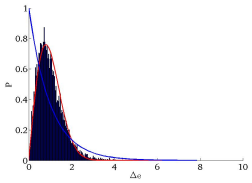
(c) V = 0.015



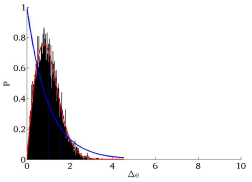
(d) V = 0.05



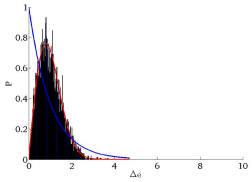
(e) V = 0.1



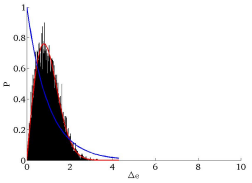
(f) V = 0.25



(g) V = 0.5

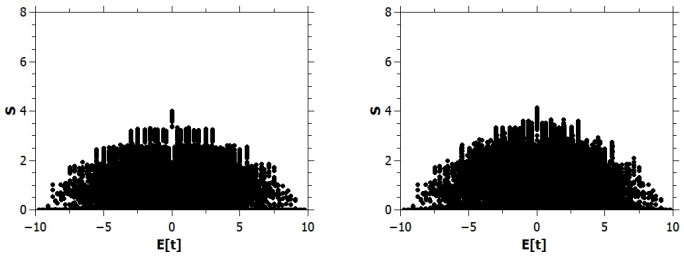


(h) V = 0.75

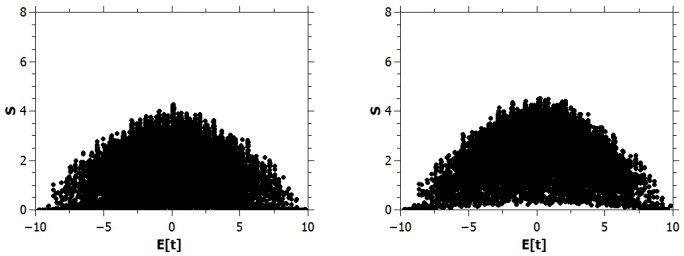


(i) V = 1

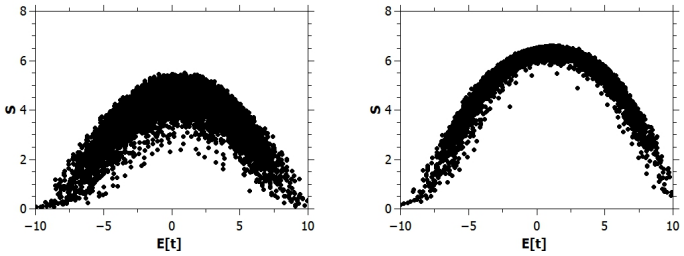
Figure 3.13: Level spacing distribution of systems with various values of V. The red curve is the Poisson distribution, the blue curve the Wigner-Dyson distribution.



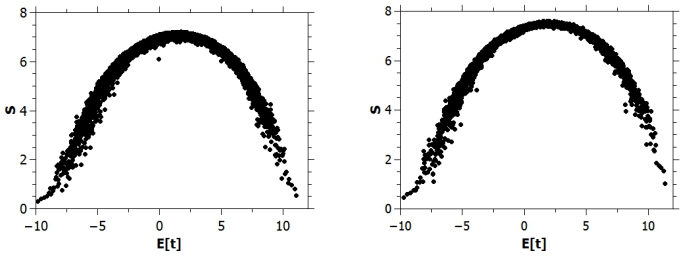
(a) V = 0.0025 (b) V = 0.015



(c) V = 0.05 (d) V = 0.1

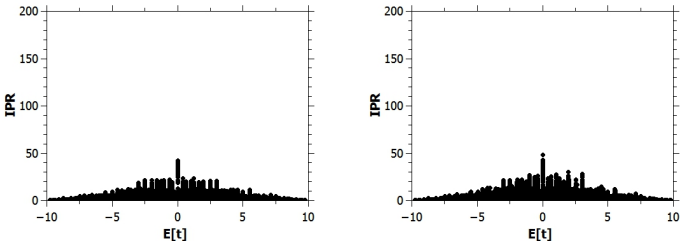


(e) V = 0.25 (f) V = 0.5



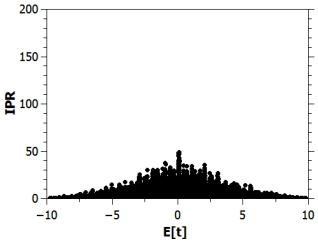
(g) V = 0.75 (h) V = 1

Figure 3.14: Shannon entropy S of the energy eigenstates with respect to the basis of the integrable model at $V = 0$ for various systems with $V \neq 0$.

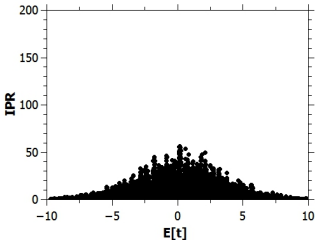


(a) V = 0.0025

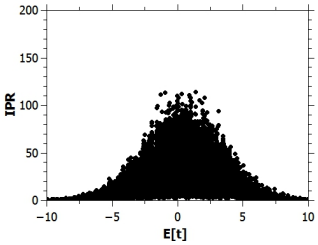
(b) V = 0.015



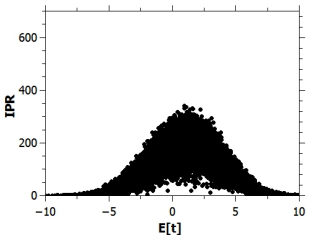
(c) V = 0.05



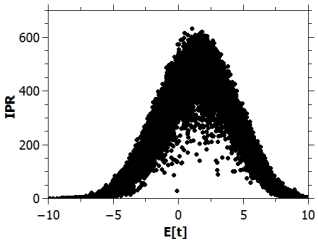
(d) V = 0.1



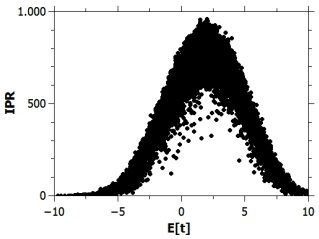
(e) V = 0.25



(f) V = 0.5



(g) V = 0.75



(h) V = 1

Figure 3.15: Inverse participation ratio (IPR) of the energy eigenstates with respect to the basis of the integrable model at $V = 0$ for various systems with $V \neq 0$.

3.6 Summary and discussion

In summary we can draw the conclusion from our results that basically all of our expectations have been met and that previously established results (mainly the ones in [5], [61]) have been confirmed.

To summarize we have studied a system of 5 spinless fermions on a $2d$ lattice very similar to the one in [5] where however hardcore-bosons were considered. As observables we have taken $n(k_x)$, which are frequently being measured in cold gas experiments and which has have also been used in other numerical studies. First we have studied equilibration of the expectation value of $n(k_x = 0)$. We have seen that the temporal fluctuations of $n(k_x = 0)$ decreased with increasing interaction strength. This was traced this back to the fact that the number of occupied energy eigenstates in the diagonal ensemble increased with increasing V, which is in accordance with Theorem 1. We have also argued that the especially large fluctuations for the system with $V = 0$ are due to the fact that it is the only system considered were the degenerate energy gap condition is not satisfied. We have then tested the second part of the eigenstate thermalization hypothesis. It was shown that the absolute values of the off diagonal elements of $n(k_x = 0)$ are significantly smaller than the diagonal ones for all values of V. They are however slightly larger for smaller interactions.Our studies were however limited by the fact that we could not increase the system sizes so that no clear conclusion can be made about equilibration. Finally we have seen that the quantum fluctuations of $n(k_x = 0)$ are very big for each time dependent state, which is due to the small sizes of the systems studied.

We have then looked at the thermalization properties of $n(k_x)$ for various values of k_x, mainly the first part of the eigenstate thermalization hypothesis. The result was that as we depart from integrability by increasing V the difference between the values of $n(k_x)$ in the diagonal and the microcanonical ensemble smoothly decreased for all k_x. We have seen that for certain values of k_x the above difference was small even for systems close to integrability. However this was due to the fact, as we have shown, that in these cases the diagonal ensemble value corresponds to an unbiased sampling and not due to the fulfilment of the ETH. To test the ETH more properly we have ploted the values of $n(k_x = 0)$ in each individual energy eigenstate. As expected with increasing interaction, for eigenstates around the center of the spectrum, the fluctuations evolve more and more into a smooth curve. We have also shown that there is a small disagreement between the predictions of the microcanonical and the canonical ensemble. This has to do with the small size of the systems considered as the equivalence of the two ensembles strictly exists only in the thermodynamic limit.

Finally the indicators of quantum chaotic behaviour were considered. First the level spacing distribution $p(s)$, which depends only on the systems spectrum, was studied. We have seen that for the integrable system at $V = 0$ there is a large peak at $s = 0$ instead of the expected Poisson-distribution. This is

due to the fact, as explained above, that there is an accidental degeneracy in the spectrum of the corresponding single particle Hamiltonian. When the interaction between the particles is turned on the level spacing distribution first resembles a Poisson curve. Upon increasing V it then smoothly evolves into the Wigner-Dyson distribution valid for Gaussian ensembles of random matrices and expected for systems far from integrability.
The second class of indicators of quantum chaos we looked at were delocalization measures of energy eigenstates with respect to some basis. The basis we have chosen is the eigenbasis of the integrable Hamiltonian with $V = 0$. We have shown that both the Shannon entropy and the inverse participation ratio evolve from strongly fluctuating behaviour throughout the whole spectrum for small V into a smooth curve and highly delocalized eigenstates around the center of the spectrum for systems with large V. The fact that away from the center large fluctuations remain indicates that delocalization measures are better indicators of quantum chaos than level spacing distributions.

In conclusion we have confirmed a smooth transition of a system from strong eigenstate to eigenstate fluctuations of observables at and close to integrability into thermal behaviour in the sense of the eigenstate thermalization hypothesis. This transitions is accompanied by a smooth transition of the energy eigenvalues and eigenstates from integrability to quantum chaotic behaviour.
The main limitation of our study is that we have not varied the system sizes, as was done for example in ref. [61]. There it is shown for $1d$ systems of bosons and spinless fermions that the transition to quantum chaos becomes faster with increasing system size, meaning that smaller integrability breaking terms are needed for larger systems. This suggests that in the thermodynamic limit thermalization might occur for infinitesimal integrability breaking terms (quantum KAM-threshold).

4 Appendix

4.1 Appendix A: proof of Theorem 1

We are now going to give a proof of Theorem 1 for the case $g((p_{E_n})_1^{d'}) = \frac{1}{d_{\text{eff}}}$ following [12]. For a proof of the other case see [10].
We will first consider a pure state $\Psi(t)$ and later extend to case of mixed states by purification. As explained in section 2.2.2 it is always possible to choose an eigenbasis $|n\rangle$ of H such that $\Psi(t)$ has finite overlap with only one state $|n\rangle$ for each distinct energy. One then has

$$\Psi(t) = \sum_n c_n \exp(-iE_n t)|n\rangle, \tag{4.1.1}$$

where $c_n = \langle n|\Psi(0)\rangle$. This time evolution (in the subspace spanned by $\{|n\rangle\}$ is equivalent to the one caused by the Hamiltonian $H = \sum_n E_n|n\rangle\langle n|$ and the time averaged state is given by

$$\omega = \sum_n |c_n|^2 |n\rangle\langle n|. \tag{4.1.2}$$

Denoting the observable by A it then follows

$$\begin{aligned}\langle|\mathrm{Tr}\{\Psi(t)A\} - \mathrm{Tr}\{\omega A\}|^2\rangle_T &= \langle|\sum_{i\neq j}(c_j^* A_{ji} c_i)\exp\{-i(E_i - E_j)t)\}|^2\rangle_T \\ &= \sum_{i\neq j, k\neq l}(c_j^* A_{ji} c_i)(c_l^* A_{lk} c_k)^* \langle\exp\{i[(E_k - E_l] - (E_i - E_j)]t)\}\rangle_T.\end{aligned} \tag{4.1.3}$$

Using the notation $\alpha = (i, j)$ and $\beta = (k, l)$ introduced in section 2.3.3 we define the vector

$$v_\beta := v_{(i,j)} := c_j^* A_{ji} c_i \tag{4.1.4}$$

and the matrix

$$M_{\alpha\beta} := \langle\exp\{i(G_\alpha - G_\beta)t)\}\rangle_T. \tag{4.1.5}$$

Using this notation eq. 4.1.3 can be written as

$$\begin{aligned}
\langle|\mathrm{Tr}\{\Psi(t)A\} - \mathrm{Tr}\{\omega A\}|^2\rangle_T &= \sum_{\alpha,\beta} v_\alpha^* M_{\alpha\beta} v_\beta \\
&\leqslant ||M||_2 \sum_\alpha |v_\alpha|^2 \\
&= ||M||_2 \sum_{i\neq j} |c_i|^2 |c_j|^2 |A_{ji}|^2 \\
&\leqslant ||M||_2 \sum_{i,j} |c_i|^2 |c_j|^2 |A_{ji}|^2 \\
&= ||M||_2 \mathrm{Tr}\{A\omega A^\dagger \omega\} \\
&\leqslant ||M||_2 \sqrt{\mathrm{Tr}\{A^\dagger A\omega^2\}\mathrm{Tr}\{AA^\dagger\omega^2\}} \\
&\leqslant ||M||_2 ||A||_\infty^2 \mathrm{Tr}\ \omega^2\} \\
&= \frac{||M||_2 ||A||_\infty^2}{d_{\mathrm{eff}}}.
\end{aligned} \tag{4.1.6}$$

The first enequality follows from the Cauchy-Schwartz inequality and the fact that the 2-norm for operators is an induced norm [22]. The third inequality is a consequence of the Cauchy-Schwartz inequality for operarors with the scalar product $\mathrm{Tr}\{A^\dagger B\}$, and the fourth follows from $\mathrm{Tr}\{P^\dagger Q\} \leqslant ||P||\mathrm{Tr}\{Q\}$, where P, Q are positive operators.
It is our aim to express $||M||_2$ in terms of $N(\epsilon)$. For this we first notice that

$$||M||_2 \leqslant \max_\beta \sum_\alpha |M_{\alpha\beta}|. \tag{4.1.7}$$

This follows from $||M||_2^2 \leqslant ||M||_1 ||M||_\infty$ and the fact that for hemitian matrices $||M||_\infty = ||M||_1 = \max_\beta \sum_\alpha |M_{\alpha\beta}|$ [22].
The matrix elements of M are

$$M_{\alpha\beta} = \begin{cases} 1 & \text{when } G_\alpha = G_\beta \\ \dfrac{\exp\{i(G_\alpha - G_\beta)T\} - 1}{i(G_\alpha - G_\beta)T} & \text{otherwise,} \end{cases} \tag{4.1.8}$$

and they satisfy $|M_{\alpha\beta}| \leq 1$.
In order to find an upper bound on the sum over α in 4.1.7 we take some arbitrary $\epsilon > 0$ and seperate the energy gap-axis in intervals of length ϵ centered symmetrically around G_β. For every integer k there are per definition $N(\epsilon)$ gaps G_α satisfying $(k + 1/2)\epsilon > G_\alpha - G_\beta \geqslant (k - 1/2)\epsilon$. Additionally for k non zero one has $|G_\alpha - G_\beta| \geqslant (|k| - 1/2)\epsilon$ and hence from eq. 4.1.8

$$|M_{\alpha\beta}| \leqslant \frac{2}{(|-1/2)\epsilon T}. \tag{4.1.9}$$

Keeping in mind that there are $d'(d'-1)$ terms in the sum $\sum_\alpha |M_{\alpha\beta}|$ one has

$$\sum_\alpha |M_{\alpha\beta}| \leqslant N(\epsilon) + 2 \sum_{k=1}^{d'(d'-1)/2} \frac{2N(\epsilon)}{(k-1/2)\epsilon T} \tag{4.1.10}$$

In ref. [12] it is shown that for $d' > 1$

$$\sum_{k=1}^{d'(d'-1)/2} \frac{1}{(k-1/2)} \leqslant 2\log_2 d'. \tag{4.1.11}$$

From this it follows that

$$||M||_2 \leqslant N(\epsilon)(1 + \frac{1 + 8\log_2 d'}{\epsilon T}. \tag{4.1.12}$$

In order to prove the theorem for mixed states we use purification. For a system with Hilbert space $\mathcal{H}$ we define a corresponding system on $\mathcal{H} \otimes \mathcal{H}$. For every initial state $\rho(0)$ on $\mathcal{H}$ there is a pure state $|\Psi(0)\rangle$ on $\mathcal{H} \otimes \mathcal{H}$ such that $\rho(0)$ is the reduced state of $|\Psi(0)\rangle$. For the Hamiltonian H and every observable A the corresponding Hamiltonian is $H \otimes \mathrm{Id}$ and the corresponding observable is $A \otimes \mathrm{Id}$, which has the same expectation value as A and satisfies $||A||_\infty = ||A \otimes \mathrm{Id}||_\infty$. Also $N(\epsilon)$ is equal for both systems as well as the effective dimension because $\mathrm{Tr}\{P_E \rho(0)\} = \mathrm{Tr}\{P_E \otimes \mathrm{Id}|\Psi(0)\rangle\}$. It is then possible to infer about the system on $\mathcal{H}$ by applying Theorem 1 to the corresponding system defined on $\mathcal{H} \otimes \mathcal{H}$.

4.2 Appendix B: Von Neumann's QET

We are now going to introduce another known concept of typicality, due to *Von Neumann* ([39], [37]), which has been applied to the thermalization of closed quantum systems. We will then discuss how these results relate to the eigenstate thermalization hypothesis. Being historically the first such approach it has been called *quantum ergodic theorem (QET)*. It is based on the concept of a macroscopic observable. For a system with Hamiltonian H we call an observable A macroscopic, if on a microcanonical Hilbert space $\mathcal{H}$ of the form $\mathcal{H}_{E,\Delta}$ (see section 2.2.6) it can be decomposed into mutually orthogonal subspaces $\mathcal{H}_\nu$ such that

$$\mathcal{H} = \bigoplus_\nu \mathcal{H}_\nu. \tag{4.2.1}$$

The subspaces $\mathcal{H}_\nu$ correspond to eigenspaces of A with eigenvalues a_ν and have huge degeneracies. We denote by $\mathcal{D}$ the family $\{\mathcal{H}_\nu\}$ and set

$$d_\nu := \dim \mathcal{H}_\nu. \tag{4.2.2}$$

Macroscopic observables can be motivated by considering a partition of the system's volume into cells that are small on the macro scale but still contain a large number of degrees of freedom [37]. Examples of observables which are

expected to be of this type are, for each cell, the density of particles, the total energy, the kinetic energy, the total momentum and the magnetization.
Von Neumann [39] argued that because the gaps between the eigenvalues of such observables will be smaller than the macroscopic resolution (which makes them highly degenerate on the macro scale), by "rounding off"(coarse-graining) such macroscopic observables one can make them into almost commuting operators on the microcanonical Hilbert space. The subspaces $\mathcal{H}_\nu$ can then be viewed as simultaneous eigenspaces of a family of commuting observables $A_1, .., A_l$ with corresponding eigenvalues characterized by a list $\nu = (a_1, ..., a_l)$ and d_ν is the degree of simultaneous degeneracy of $a_1, ..., a_l$.
Von Neumann assumed one of the macroscopic observables $A_1, .., A_l$, say A_1, to be the "macro energy", corresponding to a coarse-graining of the Hamiltonian H. This can be achieved by considering a partition of the energy axis into microcanonical intervals I_α and setting

$$A_1 := \sum_\alpha f_1(E_\alpha)|\alpha\rangle\langle\alpha|, \tag{4.2.3}$$

with the step function

$$f_1(E) := \frac{\mathcal{E}_\alpha + \mathcal{E}_{\alpha+1}}{2} \quad \text{for } E \in I_\alpha = [\mathcal{E}_\alpha, \mathcal{E}_{\alpha+1}) \tag{4.2.4}$$

Since all A_i commute, they all map $\mathcal{H}$ onto itself (recall that $\mathcal{H}$ corresponds to one energy interval I_α). As such the A_i can be regarded as operators on $\mathcal{H}$. However they in general do not correspond to conserved quantities because they commute with A_1, the macroscopic energy, but not with H.
However, motivated by the renewed interest in Von Neumann's results it has been shown that for observables $A_1, .., A_l$ with small commutators it is in general not possible to find approximation for which the commutators vanish for $l \geqslant 3$ (see [40]).

In order to formulate Von Neumann's ergodic theorem for every pure state $\Psi \in \mathcal{H}$ with $||\Psi|| = 1$ we consider the probability distribution over all macro states ν defined by the projectors P_ν onto the eigenspaces $\mathcal{H}_\nu$ of macroscopic observables, defined by

$$||P_\nu\Psi||^2 = \langle\Psi|P_\nu|\Psi\rangle \tag{4.2.5}$$

This is the probability of obtaining in a joint measurement of the observables $A_1, .., A_l$ the outcome $\nu = (a_1, ..., a_l)$. One then compares this probability distribution to the probability distribution over all macro states ν defined by the microcanonical state $\rho_{\text{mc}}[H](E, \Delta)$ on $\mathcal{H}$, given by

$$\text{Tr}\{\rho_{\text{mc}} P_\nu\} = \frac{d_\nu}{D}, \tag{4.2.6}$$

where D is the dimension of $\mathcal{H}$. In [39] (see also [37]) Von Neumann showed that for most wave functions Ψ on the unit sphere the probability distribution

over all macro states ν is close to the probability distribution defined by $\rho_{\rm mc}$. Here "most" corresponds to the uniform measure on the unit sphere of pure states in $\mathcal{H}$ (see above), such that the measure of the subset of states for which the above statement is true. Von Neumann reached this conclusion by proving for the expectation value $\mathbb{E}$ and the variance Var of $\langle\Psi|P_\nu|\Psi\rangle$ that

$$\begin{aligned}\mathbb{E}\langle\Psi|P_\nu|\Psi\rangle &= \frac{d_\nu}{D},\\ \mathrm{Var}\langle\Psi|P_\nu|\Psi\rangle &= \mathbb{E}(\langle\Psi|P_\nu|\Psi\rangle - \frac{d_\nu}{D})^2 < \frac{1}{d_\nu}(\frac{d_\nu}{D})^2.\end{aligned} \tag{4.2.7}$$

The first equation is proven using the fact that for any observable A the expectation value in the microcanonical state $\rho_{\rm mc}$ is equal to the average of $\langle\Psi|P_\nu|\Psi\rangle$ according to the uniform measure on the unit sphere in $\mathcal{H}$. This can be seen as follows:

$$\begin{aligned}\int\langle\Psi|A|\Psi\rangle\mu(\mathrm{d}\Psi) &= \int\langle n|A|n\rangle\mu(\mathrm{d}n)\\ &= \frac{1}{D}\sum_{n=1}^{D}\int\langle n|A|n\rangle\mu(\mathrm{d}n)\\ &= \int(\frac{1}{D}\sum_{n=1}^{D}\langle n|A|n\rangle)\mu(\mathrm{d}n)\\ &= \frac{1}{D}\sum_{n=1}^{D}\langle n|A|n\rangle = \mathrm{Tr}\{\rho_{\rm mc}A\},\end{aligned} \tag{4.2.8}$$

where $|n\rangle$ is some complete set in $\mathcal{H}$ and μ is the uniform measure. The above results imply that $\langle\Psi|P_\nu|\Psi\rangle$, averaged over the unit sphere in $\mathcal{H}$, gives exactly the microcanonical value $\frac{d_\nu}{D}$. At the same time the standard deviation of $\langle\Psi|P_\nu|\Psi\rangle$ from $\frac{d_\nu}{D}$ is small, provided that $d_\nu << 1$. It then follows from Chebyshev's inequality that the measure of the states for which $\langle\Psi|P_\nu|\Psi\rangle$ deviates much from the expectation value $\frac{d_\nu}{D}$ is small. This means that most states from the unit sphere give a probability distribution which is close to the microcanonical one which corresponds to the above claim.

Following Von Neumann we now make the following definition of thermalisation in a pure state.

Def.: *We call a state Ψ from the unit sphere in $\mathcal{H}$ thermal with respect to the commuting macroscopic observables $A_1, .., A_l$, if the probability distribution $\langle\Psi|P_\nu|\Psi\rangle$ is close to the microcanonical distribution defined in eq.* 4.2.6 *for every ν in $\mathcal{D}$.*

Put loosely the above typicality statement says that when looked upon macroscopically most pure states from the unit sphere look like thermal states. It is however clear that this statement cannot be true for all states, rather than most. Taking for example $\Psi \in \mathcal{H}_\nu$ for a particular ν, such a state cannot be

thermal.

The important question is now how $\langle\Psi|P_\nu|\Psi\rangle$ evolves in time if the system starts in some initial state Ψ_0. More specifically one would like to know whether

$$\langle\Psi(t)|P_\nu|\Psi(t)\rangle \approx \frac{d_\nu}{D} \tag{4.2.9}$$

for most of the time. From the above statement one can easily deduce that $\langle\Psi|P_\nu|\Psi\rangle$ will be thermal for most Ψ_0 and for most times t. However one cannot be satisfied with such a result because one expects thermal states to represent the majority, while non equilibrium states should be exceptional. Since one is mainly interested in time evolution of $\langle\Psi|P_\nu|\Psi\rangle$ from non equilibrium situations, statements about most states are not sufficient. For that reason Von Neumann's QET goes further and provides conditions under which eq. 4.2.9 holds for most initial wave functions Ψ_0. In order to formulate it properly we need the following definition [37]

Def.: *We call a macroscopic system, defined by $H, \mathcal{H}, \mathcal{D}$ and $\Psi_0 \in \mathcal{H}$, normal if and only if eq.* 4.2.9 *holds for most t. We speak of normal typicality if for most choices of $\mathcal{D}$, any macroscopic system corresponding to some fixed pair $H, \mathcal{H}$ is normal for all Ψ_0. This is equivalent to the statement that for most Hamiltonians, any macroscopic system corresponding to some fixed $\mathcal{D}, \mathcal{H}$ is normal for every Ψ_0.*

We are now ready to formulate the QET. (For a more precise formulation see [37]).

Von Neumann's QET: *Let $\mathcal{H}$ be a Hilbert space of finite dimension D, let $\mathcal{D} = \{\mathcal{H}_\nu\}$ be an orthogonal decomposition of $\mathcal{H}$ with* $\dim\mathcal{H}_\nu = d_\nu$, *and let H be a Hamiltonian on $\mathcal{H}$ which satisfies the the non-resonance condition of section* 2.2.1. *If H and $\mathcal{D}$ satisfy a technical condition, which ensures normality for energy eigenstates as initial states (see [37] for a precise formulation of this condition) then, for every initial wave function Ψ_0 from the unit sphere in $\mathcal{H}$, the system is normal. Moreover, for sufficiently large d_ν's with $\sum_\nu d_\nu = D$, most families $\mathcal{D} = \{\mathcal{H}_\nu\}$ of mutually orthogonal subspaces $\mathcal{H}_\nu$ with* $\dim\mathcal{H}_\nu = d_\nu$ *are such that the above technical condition is satisfied.*

Recently [37] have developed a modified version of Von Neumann's normal typicality. Their work is motivated by the fact that it has been shown ([41],[42]) for some reasonable choice of macro observables that among the subspaces $\mathcal{H}_\nu$ in $\mathcal{D}$ there is one particular subspace, called $\mathcal{H}_{\rm eq}$, such that

$$\frac{d_{\rm eq}}{D} \approx 1. \tag{4.2.10}$$

More precisely, the difference $1 - \frac{d_{\rm eq}}{D}$ is exponentially small in the number of particles. This implies that each observable A_i in $\mathcal{D}$ is "nearly constant" on the microcanonical shell $\mathcal{H}$. The existence of a dominant subspace $\mathcal{H}_{\rm eq}$ gives rice to a modified (with respect to Von Neumann) definition of thermal equilibrium for macroscopic observables [37].

Def.: (thermal equilibrium for observables with $\mathbf{H_{eq}}$) *We say that a state Ψ from the unit sphere in $\mathcal{H}$ is in thermal equilibrium if and only if*

$$\langle \Psi | P_{\rm eq} | \Psi \rangle = 1 - \delta, \tag{4.2.11}$$

where $P_{\rm eq}$ is the projection operator to the equilibrium subspace $\mathcal{H}_{\rm eq}$.

In reference [36] the authors are calling the set of states satisfying eq. 4.2.13 $MATE$. This definition implies that a joint measurement of the the observables $A_1, .., A_l$, which give rise to $\mathcal{D}$, will yield with probability close to 1 the equilibrium value corresponding to $\mathcal{H}_{\rm eq}$. Analogously to Von Neumann's definition of thermal equilibrium above, one can prove that most Ψ from the unit sphere are in thermal equilibrium according to this new definition. This follows from the fact, proven above, that the microcanonical density matrix can be obtained by averaging $|\Psi\rangle\langle\Psi|$ over the unit sphere. This means that

$$\begin{aligned} \int \langle \Psi | P_{\rm eq} | \Psi \rangle \mu(\mathrm{d}\Psi) = \mathrm{Tr}\{\rho_{\rm mc} P_{\rm eq}\} = \\ = \frac{d_{\rm eq}}{D} := 1 - \varepsilon, \end{aligned} \tag{4.2.12}$$

where μ is again the uniform measure. Since the quantity $\langle \Psi | P_{\rm eq} | \Psi \rangle$ is bounded from above by 1, it follows that most states Ψ must satisfy eq. 4.2.13 under the assumption that $\varepsilon << \delta$.

It is possible to prove a theorem about normal typicality along the lines of Von Neumann's QET, but using eq. 4.2.13 as definition of thermal equilibrium (see [38]). This theorem asserts that for most Hamiltonians with non degenerate eigenvalues (alternatively for most $\mathcal{D}$), $\Psi(t)$ will spend most of the time in thermal equilibrium (according to the new definition) for all initial states Ψ_0.

The concept of thermal equilibrium based on a dominant subspace $\mathcal{H}_{\rm eq}$ allows one to show that most energy eigenstates are thermal states (lie in $MATE$),again in the sense of eq. 4.2.13, and in this way to verify the ETH [36]. This is so because

$$\frac{1}{D} \sum_{n=1}^{D} \langle n | P_{\rm eq} | n \rangle = \frac{1}{D} \mathrm{Tr}\{P_{\rm eq}\} = 1 - \varepsilon. \tag{4.2.13}$$

Since $\langle n | P_{\rm eq} | n \rangle$ cannot exceed 1, most of these terms must be close to 1 under the assumption $\varepsilon << \delta$. Under the assumption that the ETH holds strictly such that all energy eigenstates are in $MATE$, it is even possible to prove a

normal typicality. Every initial state Ψ_0 will reach $MATE$ at some point in time and spend most of the time in $MATE$ in the long run (provided that H has non degenerate eigenvalues). This can be seen as follows:

$$\begin{aligned}\langle\langle\Psi(t)|P_{\text{eq}}|\Psi(t)\rangle\rangle_\infty &= \sum_{n,m}\langle\Psi_0|n\rangle\langle\exp(iE_nt)\langle n|P_{\text{eq}}|m\rangle\exp(iE_mt)\rangle_\infty\langle m|\Psi_0\rangle \\ &= \sum_n |\langle\Psi_0|n\rangle|^2\langle n|P_{\text{eq}}|n\rangle \\ &\geqslant \sum_n |\langle\Psi_0|n\rangle|^2(1-\delta) \\ &= 1-\delta,\end{aligned} \tag{4.2.14}$$

where $\langle\rangle_\infty$ refers to the infinite time average $\langle\rangle_{T\to\infty}$ (see section 2.3.1). Since it's time average is close to 1, $\langle\Psi(t)|P_{\text{eq}}|\Psi(t)\rangle$ must be close to 1 for most of the time in the long run.

One interesting aspect of the concept of $MATE$ is that the fact that most normalized pure states are in this set is true for any system. As such it is also true for so called *many body localised* systems (MBL). This are systems which have in some sense localised eigenstates, *Anderson localised* systems of particles in a random potential [43] being an example (see [45],[11] for an overview about MBL). However since these systems have vanishing transport coefficients, such that non equilibrium initial states remain out of equilibrium indefinitely, not all eigenstates can be in $MATE$. Because most energy eigenstates belong to $MATE$, such initial states must be superpositions of predominantly those eigenstates that are not in $MATE$.

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