Quantum integrable models out of equilibrium
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Chapter 1

Introduction

One of the most celebrated developments in physics is that of statistical physics, led by Maxwell, Boltzmann and Gibbs during the 19th century. Statistical physics provides a mathematical framework to make predictions for systems with a stupendous number of degrees of freedom in terms of only a few parameters. This allows us for example to understand everyday-life concepts such as temperature and pressure. Due to its predictive power and clear formulation, statistical physics is used in many disciplines of science, e.g. biology, chemistry and neurology. It may thus come as a surprising fact that, to date, very little is known in the quantum mechanical case for non-equilibrium situations. For instance, if we prepare an isolated quantum mechanical system in a specific initial state which is not an eigenstate, it is unclear under what conditions it will relax towards a state which can be described by the tools of traditional statistical physics. The aim of this thesis is to study non-equilibrium dynamics for a special class of models, quantum integrable ones. Furthermore, we address the question of the applicability of a statistical description when for these systems relaxation has occurred. We start this chapter with an overview of known results in classical mechanics and subsequently set the stage for the quantum mechanical case. All important concepts covered in this thesis will be briefly introduced, followed by an outline for the rest of the thesis.

1.1 Thermalization of classical systems

Imagine an isolated container filled with air molecules. We prepare the gas in a very specific state, for instance by compressing it into the left half of the container. If we now release the gas it will soon fill up the entire container and the air molecules will attain a Maxwell-Boltzmann speed distribution, which is up to small fluctuations constant in time. In this case we can say that the gas has thermalized. The speed distribution depends only on macroscopic quantities, which in this example are the total number of particles, the energy and the volume of the container. Microscopic details, for instance the exact state in which we prepared the gas initially in or the shape of the container, are irrelevant. The classical explanation of this is based on ergodicity. A state can be considered as a point in phase-space
1.1 Thermalization of classical systems

(restricted to the manifold of constant energy). If a system is chaotic typically the whole phase-space will be explored in time. To the phase-space one can assign a probability distribution function, which determines the probability that the system will be found in a certain infinitesimal volume of the phase-space. According to Liouville’s theorem, this phase-space distribution is conserved along the phase-space trajectories. If the system is ergodic it means, loosely speaking, that every infinitesimal volume of the phase-space is visited approximately with the same frequency over a long period of time. Assuming the ergodicity hypothesis allows us to replace time averages by phase-space averages. Such a phase-space average leads to an ensemble, that is a large number of copies of a system, considered all at once, each of which represents a possible state that the real system might be in. The ergodicity hypothesis was first introduced by Boltzmann in 1868[1]; the notion of ensembles came a decade later due to Gibbs in 1878 [2]. An example of such an ensemble is the microcanonical ensemble which describes a system where all the states have the same energy and where all states are assigned equal weights. If there are additional conserved quantities, the system is typically not ergodic and the microcanonical ensemble must be refined. This scenario will be discussed later on. The use of a statistical ensemble (which is of course completely static in equilibrium) is usually justified by the fact that a measurement always involves some sort of average over time (although it can be very short). However, it is often objected that the time to explore the entire phase-space is typically much larger than any physical time-scale and, therefore, ergodicity in the strictest sense cannot account for the validity of the use of statistical ensembles. For this reason, statistical ensembles are sometimes derived by assuming statistical independence, which was for example done by Landau in [3]. Subsystems much smaller than the entire system but sufficiently large to have macroscopic degrees of freedom are considered. Different subsystems can only interact via their boundaries. If this effect can be neglected, the subsystems can be assumed to be statistically independent. That means performing some (hypothetical) measurement in one subsystem does not affect a measurement in some of the other subsystems. Using this independence and the fact that energy for the different subsystems is additive, one can derive the canonical ensemble for the subsystems, assuming that there are no other additive conserved quantities present. The system as a whole does not need to be described by a canonical ensemble, but since an experiment typically probes only a part of the system, this is assumed to be irrelevant. In this thesis, we will discuss both views for deriving statistical ensembles in the quantum mechanical case. However, we put most emphasis on comparing time averages with statistical ensembles, since this is typically the only feasible approach for quantum mechanical systems.

Fermi, Pasta and Ulam

During the first half of the 20th century, a proof for ergodicity, for at least a specific example, was long sought after. One could naively try to solve the equations

\[ \frac{\partial \rho}{\partial t} + \sum_{i=1}^{n} \left( \frac{\partial \rho}{\partial q_i} \frac{\partial q_i}{\partial t} + \frac{\partial \rho}{\partial p_i} \frac{\partial p_i}{\partial t} \right) = 0. \]

\(^1\)Liouville’s theorem asserts for a Hamiltonian system the phase-space density \( \rho(p, q) \), which is a function of canonical coordinates \( q_i \) and conjugate momenta \( p_i \), satisfies

\[ \frac{\partial \rho}{\partial t} + \sum_{i=1}^{n} \left( \frac{\partial \rho}{\partial q_i} \frac{\partial q_i}{\partial t} + \frac{\partial \rho}{\partial p_i} \frac{\partial p_i}{\partial t} \right) = 0. \]
of motion for a specific model, but due to the enormous number of degrees of freedom required, this was intractable. This changed with the appearance of computers. Enrico Fermi, who after the war was still working in Los Alamos, had one of the first computers, MANIAC, at his disposal, which was developed to perform computations for the development of nuclear weapons. During the weekends, MANIAC was free for different types of computations. Fermi had the idea to simulate a system of many particles on the computer and to explicitly test the ergodicity hypothesis \(^2\). Nowadays this approach is very common, but in these days this way of tackling physics problems was a revolution and gave birth to computational physics. Together with Pasta and Ulam they studied a chain of particles with nearest neighbor interactions, and solved explicitly the equations of motion using MANIAC. If the interactions are purely harmonic, then of course, different vibrational modes are uncoupled so there will be no ergodicity. However, it was believed that a non-linear force (leading to non-linear differential equation) would guarantee ergodicity. For a chain of \(N = 32, 64\) particles prepared in a specific state they studied the time evolution for various non-linear interactions (by adding quadratic or cubic forces). At first, everything seemed in complete agreement with common intuition. However, one weekend they forgot to switch off the computer and discovered quasi-periodic motion. Initially, the accuracy of the numerics was questioned, and also the possibility of Poincaré recurrences \(^3\) was considered, which were known to occur in ergodic systems. Further analysis excluded both potential explanations, and the results where eventually published without explanation in 1955 \([4, 5]\) \(^4\) just after Fermi’s death.

**Integrability and the KAM theorem**

For a possible explanation of the FPU problem we need to introduce two concepts: integrability and the KAM theorem. Although the system considered by Fermi, Pasta and Ulam contained non-linear interactions, its continuum version is described by the integrable Korteweg-deVries equation, which they did not realize. A classical system with \(n\) degrees of freedom (i.e. with \(2n\)-dimensional phase-space) is called *integrable* if it possesses \(n\) independent first integrals of motion in involution (i.e. Poisson-commuting); see also chapter 4. Such a system is integrable in the sense that in terms of action-angle variables the differential equations describing the time evolutions can be explicitly integrated. The solutions of the equations of motion thus display periodic motion on tori in phase-space, and ergodicity is absent. The quasi-periodic motion observed by FPU can now be explained using the KAM theorem \([6, 7, 8]\). The KAM theorem states that if the system is subjected to a weak nonlinear perturbation, some of the invariant tori are deformed and survive, while others are destroyed. This implies that the motion continues to be quasiperiodic on part of the phase-space of positive measure. The KAM theorem specifies what level of perturbation can be applied for this to be

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\(^2\) Actually they studied equipartitioning of the different vibrational models, which happens only when the system is ergodic.

\(^3\) The Poincaré recurrence theorem states that isolated systems will, after a sufficiently long time, return to a state very close to the initial state.

\(^4\) Many years after the publication it became clear that actually most of the numerical work was done by Mary Tsingou who was for mysterious reasons not mentioned as an author.
true. An important consequence of the KAM theorem is that for a set of initial conditions, with positive measure, the motion remains perpetually quasiperiodic. Non-integrable models that fall into this class are, therefore, non-ergodic. In fig. 1.1 an artist’s impression is shown of the KAM theorem.

Figure 1.1: An artist’s impression of the KAM theorem. The cube illustrates the phase-space (restricted to constant energy) with trajectories for: an integrable model (left), quasi-integrable model (middle) and a chaotic model (right). Only in the last case does one expect ergodicity.

The models studied by Fermi, Pasta and Ulam were close to integrable, however it is difficult to rigorously prove that the KAM theorem accounts for the observed absence of ergodicity. Nevertheless, the KAM theorem tells us that, although integrable models are very special, they are still very important to study.

1.2 Thermalization of quantum systems

Thermalization for isolated quantum many-body systems is a completely different story, as was already realized by von Neumann in 1929 [9]. The most important difference is that there is no quantum analog of a phase-space. Instead, quantum mechanical states are defined as vectors in a Hilbert space. Furthermore, the counting of the degrees of freedom is completely different for classical and quantum mechanical systems. These are some of the reasons why we cannot easily define a quantum mechanical version of integrability in the Liouville sense. Chapter 4 is completely devoted to defining quantum integrability, and we give only a working definition for now: a quantum mechanical system is integrable\(^5\) if there is a set of conserved charges \(\{Q_i\}\) which is unbounded in the thermodynamic limit, and the conserved charges mutually commute. Another difference is that for isolated quantum mechanical systems we have unitary time evolution. Suppose the system at \(t = 0\) is in the state \(|\psi_0\rangle\). The subsequent time evolution is then simply

\[
|\psi(t)\rangle = e^{-iHt} |\psi_0\rangle = \sum_n c_n |n\rangle e^{-iE_n t} \quad c_n = \langle n | \psi_0 \rangle, \tag{1.1}
\]

where the sum is over all eigenstates \(|n\rangle\). The coefficients \(c_n\) are assumed to be normalized: \(\sum_n |c_n|^2 = 1\). For a finite number of degrees of freedom, the

\(^5\)Where possible, we will shorten quantum integrability to integrability.
system generically shows a periodic (or quasi-periodic) behavior with a period that typically increases rapidly when the number of degrees of freedom grows. This (quasi-)periodic behavior is the well-known phenomenon of quantum recurrence. Von Neumann formulated a necessary and sufficient condition for a macroscopically large system to relax: the absence of resonances \[9\], i.e.

\[
E_m - E_n \neq E_{m'} - E_{n'} \text{ unless } \begin{cases} 
\text{either } m = m' \text{ and } n = n' \\
\text{or } m = n \text{ and } m' = n'.
\end{cases}
\]

In practice, this condition turns out to be too strong: as long as it is only violated for a sufficiently small number of energy levels the system typically will still relax. We can now ask the following question:

Given that a system relaxes, can it be described by a statistical ensemble?

It is useful to first formulate the problem in terms of density matrices. Instead of \[(1.1)\] we can write

\[
\rho(t) = \sum_{m,n} c_m^* c_n |n\rangle\langle m| e^{i(E_n - E_m)t}.
\]

The large time limit \((t \to \infty)\) of this density matrix is not well-defined, we therefore introduce a time average

\[
\bar{\rho} \equiv \lim_{T \to \infty} \frac{1}{T} \int_0^T \rho(t) dt = \rho_{\text{diag}} + \rho_{\text{offdiag}}
\]

\[
= \sum_n |c_n|^2 |n\rangle\langle n| + \sum_{m \neq n} c_m^* c_n |m\rangle\langle n| \delta_{E_m, E_n}.
\]

The second term is due to possible degeneracies in the spectrum but can typically be neglected, even in cases where the system is quantum integrable. However, counter examples do exist, for instance when in the thermodynamic limit the density of states is diverging or discontinuous. Such an example is discussed in chapter 5. In the literature, \(\rho_{\text{diag}}\) is called diagonal ensemble \[10\]. We can now try to formulate a quantum ergodic theorem. Since quantum mechanically there is no notion of phase-space, the formulation is less precise and intuitive. Let us first of all define a quantum microcanonical density matrix: given a Hamiltonian with eigenstates \(|n\rangle\) with energies \(E_n\), the microcanonical ensemble is obtained by coarse-graining the spectrum on energy shells of width \(\Delta E\), sufficiently big to contain many states but small on macroscopic scales. Then the microcanonical density matrix for a given energy \(E\) is

\[
\rho_{\text{mic}}(E) = \sum_{E \leq E_n < E + \Delta} \frac{1}{\mathcal{N}} |n\rangle \langle n|
\]

with \(\mathcal{N}\) the number of states in the shell \([E, E + \Delta)\). If we prepare a state \(\rho_{\text{diag}}\) constrained to a microcanonical shell, the most obvious definition of ergodicity, \(\rho_{\text{diag}} = \rho_{\text{mic}}\), implies that \(|c_n|^2 = 1/\mathcal{N}\) for all \(n\). Quantum ergodicity in this strict sense is therefore almost never realizable \[9, 11\]. The key to understanding thermalization of isolated quantum systems is to shift the focus on observables...
1.2 Thermalization of quantum systems

rather than on the states themselves. In his paper, von Neumann starts from the following reasoning: “In a macroscopic measurement of coordinate and momentum (or two other quantities that cannot be measured simultaneously according to quantum mechanics), really two physical quantities are measured simultaneously and exactly, which however are not exactly coordinate and momentum. They are, for example, the orientations of two pointers or the locations of two spots on photographic plates and nothing keeps us from measuring these simultaneously and with arbitrary accuracy, only their relation to the really interesting physical quantities is somewhat loose, namely the uncertainty of this coupling required by the laws of nature corresponds to the uncertainty relation.” This motivated him to construct a set of commuting macroscopic observables \( \{M_\alpha\} \), coarse-grained onto the microcanonical shell. The set of \( \{M_\alpha\} \) is obtained by starting from a set of macroscopic operators and “rounding them off” in order to make them commute. Assuming some conditions, von Neumann proved for these commuting macroscopic observables the so-called quantum ergodic theorem [9]. Recently, the quantum ergodic theorem was re-examined in [11] where the authors summarize the result by von Neumann as follows: “for a typical finite family of commuting macroscopic observables \( \{M_n\} \), every initial wave function \( |\psi_0\rangle \) from a microcanonical energy shell so evolves that for most times \( t \) in the long run, the joint probability distribution of these observables obtained from \( |\psi(t)\rangle \) is close to their microcanonical distribution.” Although this result is very general, one is typically interested in the time-evolution of a very specific observable, for example a correlation function that can be probed in experiments. For this reason, we will omit in this thesis a more detailed discussion of von Neumann’s work, and will instead present explicit examples of observables.

The observables one is usually interested in are typically constructed as a finite product of local operators, so-called \( n \)-point functions. We will denote these observables by \( O(x) \), where \( x \) is a set of arbitrary parameters which can be for example position, time or distance between operators. The time evolution for the expectation of \( O(x) \) is given by

\[
\langle O(x,t) \rangle = \sum_{m,n} c_n^* c_m \langle m|O(x)|n \rangle e^{i(E_m - E_n)t} \tag{1.6}
\]

and the corresponding time average is

\[
\langle O(x) \rangle = \sum_n |c_n|^2 \langle n|O(x)|n \rangle + \text{off-diagonal matrix elements}. \tag{1.7}
\]

Assuming that the off-diagonal terms are negligible and that the distribution \( |c_n|^2 \) is sufficiently narrow in energy, one can ask ourselves under what conditions can the time average of \( O(x) \) be described by a microcanonical ensemble, i.e.

\[
\sum_n |c_n|^2 \langle n|O(x)|n \rangle \approx \sum_{E \leq E_n < E+\Delta} \frac{1}{N} \langle n|O(x)|n \rangle. \tag{1.8}
\]

Following [10] we can think of three scenarios for which the above equality holds:

1. The coefficients \( c_n \) are constant for equal energies within the energy band.
2. The expectation values $\langle n|O(x)|n \rangle$ are approximately constant over the interval $[E, E + \Delta]$.

3. The fluctuations in the coefficients $c_n$ and expectation values $\langle n|O(x)|n \rangle$ are uncorrelated.

The first scenario we already rejected in the discussion of quantum ergodicity since for most initial states this will be false. The second scenario is the eigenstate thermalization hypothesis (ETH) which was proposed by Deutsch and Srednicki [12, 13]. The ETH gives a very different explanation for the thermalization compared to the classical case. According to the ETH, every eigenstate always implicitly contains a thermal state, the coherence between the eigenstates initially masks it but time evolution reveals it through dephasing (see fig. 1.2). There is no general proof of the ETH, however there exist various semi-classical arguments. For instance in [13], thermalization of a quantum gas with hardcore interactions was studied. It was found that if the initial condition $|\psi_0 \rangle$ is sufficiently narrow in energy and Berry’s conjecture\(^6\) [14] is obeyed, the momentum distribution will always relax to the Maxwell-Boltzmann distribution. The ETH has also been numerically verified for various models that can be regarded as far from integrable [10, 15, 16]. For an integrable model one can imagine that the expectation value is a smooth function not only of energy but also of all the other conserved charges and therefore the ETH will not hold. It should be noted that the ETH clearly does not hold for every observable.

In the third scenario the fluctuations of the overlaps $c_n$ and the expectation values $\langle n|O(x)|n \rangle$ are uncorrelated, in which case the initial state performs an unbiased sampling of the distribution of expectation values. An example where this scenario turned out to be responsible for thermalization was investigated in [17]. There, the initial state was prepared in a non-integrable model, while the time evolution was governed by an integrable system.

In the literature typically only the three scenarios discussed above are considered to explain thermal behavior as in (1.8), however we would like to stress that the number of possible scenarios is not limited to these three.

### 1.3 Cold Atomic Gases

Until a few years ago, the questions related to isolated quantum systems out of equilibrium would have been completely academic. However, with the recent advances in the field of ultra cold atomic gases it is possible to experimentally construct many-body systems that can be viewed as (almost) isolated systems. Furthermore, these gases are highly controllable; for example via Feshbach resonances the interaction strength can be controlled to realize both weakly and strongly interacting many-body systems. Moreover, one can superimpose an external potential, thereby reducing the dimensionality and/or creating an optical lattice. One system of particular importance for this thesis is the quai-one-dimensional Bose gas

\(^6\)Berry’s conjecture is expected to hold only if the corresponding classical system is chaotic, and essentially states that the eigenstates $|n \rangle$ can be considered as pseudorandom superpositions of plane waves.
1.3 Cold Atomic Gases

Figure 1.2: Left: thermalization in classical systems due to chaos. Right: according to the ETH, each state can be considered as a thermal state in the sense that different eigenstates in the same energy shell yield equal expectation values for local observables. The thermal behavior can be initially hidden by the coherence of the eigenstates, but through dephasing it will be revealed. Picture taken from \[10\].

which can be described by the integrable Lieb-Liniger model which we will discuss in chapter 2 and has experimentally been realized in various circumstances \[18, 19, 20, 21\]. For a review of this fast emerging field we refer to \[22\]. Below, we will discuss two exemplary experiments which studied quantum gases out of equilibrium.

**Collapse and revival of a matter wave**

In \[23\], a Bose gas on a cubic lattice is constructed. The system can approximately be described by the Bose-Hubbard model

\[
H = -J \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_i a_j^\dagger) + \frac{U}{2} \sum_i n_i(n_i - 1). \quad (1.9)
\]

Here, the first term describes hopping of bosons to nearest neighbor sites and the second term is the on-site repulsion between the bosons. When \(J \gg U\), the system behaves as a superfluid while in the opposite limit, \(U \gg J\), the system is in the Mott insulating phase. The experiment \[23\] initially prepared the system in the superfluid phase, followed by a sudden change (quantum quench) of the on-site repulsion \(U\). The Hamiltonian after the quench is approximately \(H = \frac{U}{2} \sum_i n_i(n_i - 1)\). Since the energy levels of the final Hamiltonian are integer multiples of \(U\), the revival time of the wavefunction is simply \(t_{\text{rev}} = 1/U\).
The absorption images\textsuperscript{7} for various $t = 0, \ldots, t_{\text{rev}}$ are shown in fig. 1.3, the colors are proportional to the density of bosons. In frame $a$) the system is in the superfluid phase, the bright peaks corresponds to the coherently occupied momentum modes. The coherence is completely lost in frame $d$), where no interference pattern is visible at all, but is later almost completely restored at $t = t_{\text{rev}}$ in frame $g$). This experiment clearly demonstrates the unitary time evolution for quantum many-body systems can be visualized experimentally, and that the experimental time scales are sufficiently long to study non-equilibrium dynamics.

\textbf{A quantum Newton’s cradle}

Another remarkable experiment on non-equilibrium physics was performed in [18]. Interacting bosons are loaded in a one-dimensional harmonic trap. When the trap is sufficiently flat, this setup can approximately be described by the integrable Lieb-Liniger model, which we will discuss later on in this thesis. By applying two Bragg pulses shortly after each other, the gas is split into two clouds of opposite momenta. As a result, the two clouds start to oscillate in the harmonic potential and collide when they are both in the center of the trap. The momentum distribution after a full cycle is shown in fig. 1.4. Due to the anharmonicity, the momentum distribution becomes stationary after a while, but is different from a thermal one. As a possible explanation for the absence of thermalization, it was first proposed that the model is sufficiently close to a quantum integrable model,

\footnote{The absorption images are obtained by suddenly turning off all confining potentials allowing the bosons to freely expand and interfere with each other. After a fixed hold time the density of the bosons is measured in real space.}
but this has not been verified yet. One can also imagine that for this specific setup the two clouds only interact via 2-body scattering processes, which in one dimension is insufficient for thermalization because of conservation of energy and momentum. Although the individual clouds might thermalize, the system as a whole will not, irrespective of whether the system is integrable or not. For comparison, the experiment was also repeated in three dimensions where they found that a thermal state was obtained after approximately three oscillations. In this case both explanations given above do not apply. Although this experiment received a considerable amount of attention, it is fair to say that, to date, it is still not completely understood.

Figure 1.4: \textit{Left}: a sketch of the quantum's Newton cradle experiment. At $t = 0$ the atoms are prepared as a superposition of opposite momenta. The two clouds start to oscillate and collide twice every full cycle of period $\tau$. \textit{Right}: the absorption images, corresponding to the momentum distribution, for a full cycle. Images taken from [18].

1.4 Quantum Quenches

There are various ways to prepare a system in an initial state $|\psi_0\rangle$ such that subsequent time evolution results in non-equilibrium dynamics. One important example, both theoretically and experimentally, is a so-called quantum quench. At $t = 0$, the system is in the ground state $|\psi_0\rangle$ of a Hamiltonian $H_0$. Then at $t > 0$ we instantaneously change some parameter of the Hamiltonian, thus obtaining a different Hamiltonian $H$ such that $[H_0, H] \neq 0$. The state after the quantum quench is then simply $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$. In this thesis we will focus mainly on quantum quenches.

One of the first examples of a quantum quench that was studied is the XY-Ising chain in a transverse field [24, 25, 26]. Using the mapping to free fermions, the time evolution of the transverse magnetization after an instantaneous change of
the external transverse field was computed exactly. Similar investigations followed since then, mainly for models that can be mapped to an effectively free Hamiltonian (see for example [27, 28, 29, 30]). However, from these case-by-case studies it was hard to extract a general physical picture for the relaxation correlation functions after a quench.

Much progress was made by Calabrese and Cardy, who studied quantum quenches where the post-quench Hamiltonian describes a conformal field theory (CFT). In their arguments they use a path integral approach and the well-known mapping of the quantum problem to a classical one in $d+1$ dimensions. The initial state $|\psi_0\rangle$, which is the ground state of the Hamiltonian $H_0$ with a mass gap $m_0$, plays the role of a boundary condition. In case of the 1+1 dimensional problem, powerful techniques of boundary conformal field theory can be applied to study the time evolution of the entanglement entropy [31] as well as correlation functions [32, 33]. For the relaxation of a primary field operator $\Phi$, they found

$$\langle \Phi(t) \rangle \propto e^{-x\pi t/2\tau_0},$$

$$\langle \Phi(r,t)\Phi(0,t) \rangle - \langle \Phi(0,t) \rangle^2 \propto \begin{cases} 0 & \text{for } t < r/2, \\ e^{-x\pi r/2\tau_0} - e^{-x\pi t/\tau_0} & \text{for } t > r/2, \end{cases}$$

where $\tau_0$ is a non-universal constant and $x$ is the scaling dimension of $\Phi(r)$. Their findings allowed a simple interpretation in terms of classical quasi-particles. The initial state $|\psi_0\rangle$ has an (extensively) high energy relative to the ground state of the Hamiltonian $H$, which governs the subsequent time evolution, and therefore acts as a source of quasi-particle excitations. Those quasi-particles originating from closely separated points (roughly within the correlation length $\xi_0$ of the ground state of $H_0$) are quantum entangled and particles emitted from points far away from each other are incoherent. If the quasi-particle dispersion relation is $E = \omega_k$, the classical group velocity is $v_k = \partial_k \omega_k$. We assume that there is a maximum speed $v_m = \text{max}_k |v_k|$. A quasi-particle of momentum $k$ produced at $r$ is therefore at $r + v_k t$ at time $t$, assuming scattering effects can be ignored. These free quasi-particles have two distinct effects. Firstly, incoherent quasi-particles arriving at a given point $r$ from well-separated sources cause relaxation of (most) local observables. Secondly, entangled quasi-particles arriving at the same time $t$ at points with separation $|r| \gg \xi_0$ induce quantum correlations between local observables. In the case where they travel at a unique speed $v$ (as is the case for a CFT), therefore, there is a sharp “horizon” or light-cone effect: the connected correlations do not change from their initial values until time $t \sim |r|/2v$. After this time, they rapidly saturate to time-independent values. For large separations (but still much smaller then $2vt$), these decay exponentially.

Still, the study of non-equilibrium problems remains a theoretical challenge. One approach is the use of numerical algorithms such as time-dependent density matrix renormalization group (tDMRG) (e.g. [34, 35]) and the time-evolving block decimation (TEBD) algorithm (e.g. [36, 37]). Although these methods can be applied to a wide range of problems, they suffer from the fact that the inaccuracy of their results increases in time, which makes the large time limit inaccessible and these methods are therefore not suitable to study for instance thermalization. A recent line of development is to use integrable field theories for quantum quenches.
1.5 The Generalized Gibbs Ensemble

[38, 39, 40]. This looks very promising, although, to date, there are no examples of the time evolution of fully interacting theories. The method we will use in this thesis is the algebraic Bethe ansatz, which will be discussed in chapter 3. The algebraic Bethe ansatz was developed for the computation of correlation functions of certain integrable models. For dynamical correlation functions in a finite volume, this method, combined with numerics, proved to be extremely powerful [41]. Recently, this approach has also been applied to quench problems [42, 43]. One of the aims of this thesis is to further develop this direction.

1.5 The Generalized Gibbs Ensemble

As discussed earlier in this chapter, it is expected that quantum integrable models generically do not thermalize. The conventional statistical ensembles typically do not apply, since now not only the total number of particles and energy are important macroscopic quantities, but the higher conserved charges might play an important role as well. Inspired by Jaynes’ maximum entropy argument [44], Rigol et. al. proposed the generalized Gibbs Ensemble (GGE) [27] in which all ‘relevant’ conserved charges \{\hat{Q}_j\} are included

\[ \rho_{\text{GGE}} = \frac{1}{Z_{\text{GGE}}} e^{-\sum_n \beta_n \hat{Q}_n}. \]  

(1.12)

with \( Z_{\text{GGE}} = \text{Tr}\{e^{-\sum_n \beta_n \hat{Q}_n}\} \). The set of Lagrange multipliers\(^8\) \( \beta_n \) are fixed via the initial conditions

\[ \langle \psi_0 | Q_j | \psi_0 \rangle = \text{Tr}\{Q_j \rho_{\text{GGE}} \}. \]  

(1.13)

Once all the \( \beta_j \) are determined, one can compute the expectation value of an observable \( O(x) \) in the usual way: \( \langle O(x) \rangle_{\text{GGE}} = \text{Tr}\{O(x) \rho_{\text{GGE}} \} \). The GGE is particularly useful for quantum quenches, since in this case the initial state is known, from which the \( \beta_j \) can in principle be derived. The upshot of this is that, if the GGE is valid, expectation values for the large time limit can be computed without the need of computing the time evolution, which is typically very complicated. On the other hand, if for instance a Hamiltonian parameter is gradually changed, the conserved charges change as well during this process, which makes it hard to determine the \( \beta_j \) since one has to compute the time evolution in some way to make predictions for late times.

1.5.1 Maximum entropy estimates

In order to motivate the GGE, we follow Jaynes’ maximum entropy argument [44], which is based on information theory. Consider a system with a large number \( n \) of possible states, \( |\psi_i\rangle \), with corresponding probabilities \( p_i \). We assume that the probabilities are normalized: \( \sum_i p_i = 1 \). Expectation values are computed as \( \langle O(x) \rangle = \sum_i p_i \langle \psi_i | O(x) | \psi_i \rangle \). In general one does not know the microscopic data \( p_i \) of a physical system. Suppose that we know \( m \ll n \) expectation values

\(^8\)The Lagrange multiplier \( \beta_n \) are sometimes also called generalized chemical potentials or generalized inverse temperatures.
\[ E^{(j)} = \sum_i p_i \langle \psi_i | A^{(j)} | \psi_i \rangle \] instead. Now we can ask on the basis of this given information what is the expectation value of an observable \( O(x) \)? Here we assume that \( O(x) \) cannot be decomposed into \( A^{(j)} \). At first glance, this might seem a meaningless question since the number of unknowns \( n - m - 1 \) is large. But if we are optimistic and want to make a prediction anyway, can we do this without any bias? Putting it differently, we want to make predictions with maximal uncertainty constraint to the information we have. Requiring that the measure for uncertainty is positive, increases with increasing uncertainty, and is additive for independent sources of uncertainty, one can prove that there is a unique measure which is called Shannon’s entropy \[ S = - \sum_i p_i \ln p_i. \] (1.14)

In the physics literature \( S \) is also known as the Gibbs entropy (after multiplying with Boltzmann’s constant)\(^9\). The case where we have no information about the expectation values, maximizing the entropy leads to the distribution \( p_i = 1/n \); which one can recognize as the microcanonical ensemble for a closed system. If we know a single expectation value \( E = \sum_i p_i \langle \psi_i | A | \psi_i \rangle \) we can maximize the entropy (1.14) by introducing a Lagrange multiplier \( \beta \), leading to

\[ p_i = \frac{e^{-\beta A_i}}{Z}, \quad A_i = \langle \psi_i | A | \psi_i \rangle, \] (1.15)

which we recognize as the Boltzmann factors defining the canonical ensemble. The partition function \( Z \) is fixed by \( Z = \sum_i e^{-\beta A_i} \) and the Langrange multiplier \( \beta \) is determined via \( E = \sum_i e^{-\beta E_i} E_i / Z \). Using the same arguments, the maximum entropy distribution in case of \( m \) known expectation values \( E_j \) is simply

\[ p_i = \frac{e^{-\sum_{j=1}^m \beta_j A_i^{(j)}}}{Z}. \] (1.16)

The above reasoning is not restricted to conserved charges, but since we want to avoid having to compute some sort of time evolution, conserved charges are the only sensible choice. In chapter 4 we will give some criteria for which conserved charges are expected to be important for constructing the GGE.

### 1.5.2 Results for the generalized Gibbs ensemble

The GGE has proved successful on many occasions, by comparing it with the long time average of specific observables. In one of the first examples \[27\], the momentum distribution of hard-core bosons on a lattice, after release from a trap, was studied numerically. Other numerical tests are \[46, 28, 47\]. One of the first exactly solved quench problems where the GGE was proven to be correct was for a chain of coupled harmonic oscillators \[33\]. In chapter 7 we will further analyze this example. Other exact studies for free models focusing on subsystems rather than on observables are \[48, 49\]. For integrable field theories and specific initial states, the density matrix in the infinite time limit was shown to be of the GGE

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9A related quantity is the von Neumann entropy which is defined in terms of the density matrix \( \rho \) for a quantum mechanical model: \( S = -\text{Tr}(\rho \ln \rho) \).
form [38]. An interesting observation is that for certain integrable models, the large time limit for certain observables can be described with just a canonical ensemble rather than a GGE. In a first numerical study for the transverse Ising model, in which the transverse field was suddenly changed, the two-point function of the order parameter looked thermal [29]. An exact study of the same problem [30], revealed that the long time average for this observable is always described by the GGE, but for a certain range of parameters the canonical ensemble provides a good approximation. Another instance in which the large time limit looks thermal are the correlation functions of primary fields of a 1+1 dimensional CFT studied in [33]. Although the system is integrable, the specific choice of initial state yields a thermal-like behavior. Despite all the successes there are also examples where the GGE fails. When for instance translational invariance is broken in the initial system, certain expectation values are not correctly predicted by the GGE [50, 51]. Another example is discussed in chapter 6 where we study a quench for bosons and observe that the GGE fails; this is cured by introducing the generalized canonical ensemble. However, in the thermodynamic limit the two ensembles are expected to coincide.

1.6 Outline

In the next two chapters we introduce the most important tool used in this thesis, the Bethe ansatz. We start chapter 2 with a discussion of what wavefunctions in one dimension might look like, followed by the so-called coordinate Bethe ansatz for wavefunctions of the Lieb-Liniger model and the XXZ spin chain. Although the coordinate Bethe ansatz is quite useful for gaining an intuitive understanding, for actually computing correlation functions and for studying quench problems we need the algebraic Bethe ansatz presented in 3. In chapter 4, we discuss the notion of quantum integrability and introduce a new definition, leading to a classification of integrable models [52]. We change gears in the following two chapters by studying the time evolution after two types of quantum quenches. Chapter 5 deals with the problem of a spin chain, initially prepared in a spatially inhomogeneous (domain wall) state, where subsequent time evolution is governed by the XXZ chain [53]. In chapter 6, we study the case where the system is initially in the ground state of the fully interacting Lieb-Liniger model. The quench consists of instantaneously switching the interactions off [54]. A more formal discussion of equilibrium states (e.g. the large time limit after a quantum quench) is presented in chapter 7 where we introduce the generalized thermodynamic Bethe ansatz [55]. We end with a conclusion of our results and discuss possible directions for future research.