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Halil Cakir

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Dynamics of the Transverse Field Ising Chain after a Sudden Quench

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Dynamik der Ising-Kette in einem transversen Feld nach einem plötzlichen Quench:

Wir betrachten die Dynamik der longitudinalen Spin-Korrelationsfunktion nach einem plötzlichen Quench in der Ising-Spin-Kette in einem transversen Feld. Es wird eine detaillierte Herleitung des Spektrums des Modells präsentiert, indem gezeigt wird, dass der Hamilton-Operator des Systems sich als ein Hamilton-Operator nicht-wechselwirkender Fermionen schreiben lässt. Dadurch ist man im Stande durch die Anwendung des Wick'schen Theorems die longitudinale Spin-Korrelationsfunktion für Systeme beliebiger (aber endlicher) Größe zu bestimmen. Des Weiteren wird beobachtet, dass im thermodynamischen Limes die Dynamik nach asymptotisch langen Zeiten nach dem plötzlichen Quench zu stationären Werten führt, die sich durch ein geeignetes verallgemeinertes Gibbs'sches Ensemble beschreiben lassen. Insbesondere konzentrieren wir uns auf die Dynamik des longitudinalen Korrelators nach einem plötzlichen Quench von einem anfangs großen externen Feld in die Nähe des quanten-kritischen Punktes innerhalb der paramagnetischen Phase. Basierend auf asymptotischen Ausdrücken in [Calabrese et al., 2012a] wird eine verbesserte Formel vorgeschlagen und diese wird mit numerischen Rechnungen verglichen. Dabei wird beobachtet, dass der Zerfall der Korrelationfunktion durch zwei Korrelationslängen charakterisiert ist. Insbesondere wird festgestellt, dass die Korrelationsfunktion ihre stationären Werte bereits auf sehr kurzen Distanzen annimmt.

Dynamics of the Transverse Field Ising Chain after a Sudden Quench:

We study the dynamics of the longitudinal spin correlation function after sudden quenches in the Ising chain in a transverse field. We give a detailed derivation of the spectrum of the model by showing that the Hamiltonian of the system can be expressed as a Hamiltonian of non-interacting fermions. This enables us to determine the longitudinal spin correlation function for chains of any (finite) size by using Wick's therorem. We find that, in the thermodynamic limit, the dynamics leads to stationary values given by an appropriately defined generalized Gibbs ensemble for asymptotically large times after the sudden quench. In particular, we concentrate on the dynamics of the longitudinal correlator after sudden quenches from initially large external fields to the vicinity of the quantum critical point within the paramagnetic phase. Based on asymptotic expressions given in [Calabrese et al., 2012a], we conjecture a new formula and compare it to our numerical calculations. With that, we find that the decay of the correlation function is characterized by two correlation lengths. In particular, we observe that the correlation function attains its stationary values already at short distances.

Contents

1 Introduction

Nowadays, experimental advances in the preparation and control of ultra-cold atomic gases allow to observe the behaviour of isolated quantum systems out of equilibrium for long timescales [Kinoshita et al., 2006, Greiner et al., 2002, Trotzky et al., 2012]. These systems are weakly coupled to their environment and, thus, the thermalization due to dissipation is minimal. Therefore, they provide an ideal testing ground for theoretical ideas regarding unitary non-equilibrium dynamics.

In these systems, one is interested in the time dependence of observables. In particular, it is important to understand whether the non-equilibrium dynamics can lead to stationary values for the observables and, if it does, whether these values can be described by an appropriately chosen ensemble. So-called sudden quenches are the most common way to probe an isolated quantum system for this question in experiment. A sudden quench is an abrupt change of the parameters of the Hamiltonian describing the dynamics of the isolated quantum system.

In [Rigol et al., 2007], it has been conjectured that, for sudden quenches in integrable quantum systems, the observables attain stationary values which can be described by a so-called generalized Gibbs ensemble [Jaynes, 1957a,b]. A generalized Gibbs ensemble is a generalization of the usual (thermal) Gibbs ensemble which is obtained by maximizing the von Neumann entropy under the constraint that there are other conservation laws besides the one for the energy. In fact, generalized Gibbs ensemble are not only a theoretical concept but have been observed experimentally in [Langen et al., 2015].

The conjecture put forward in [Rigol et al., 2007] has been analysed for some integrable quantum systems. The authors themselves considered the dynamics of hard-core bosons numerically and confirmed their conjecture.

Among those integrable quantum systems is the transverse field Ising chain. This model describes spin-1/2 systems where the spins in the x-direction interact with their nearest-neighbours and with an external field in the z-direction. A distinguishing feature of this model is that it admits a quantum phase transition, which is considered to be a phase transition at zero temperature. The system has a quantum critical point which separates a ferromagnetic phase from a paramagnetic phase.

The transverse field Ising chain is a special case of the more general XY model in which also the spins in y-direction interact with their nearest-neighbours. The spectrum of the XY chain without an external transverse field and the spin correlations in the ground state have been first determined in [Lieb et al., 1961] by introducing fermionic degrees of freedom. Based on this work, the XY chain in a transverse external field has been diagonalized in [Katsura, 1962] and its thermodynamical quantities have been analysed in [Barouch et al., 1970, Barouch and McCoy, 1971a,b, McCoy et al., 1971]. Since the transverse field Ising chain is a special case of the XY chain, corresponding calculations can be performed using the same methods. In fact, the transverse field Ising chain has been directly diagonalized in [Pfeuty, 1970].

Sudden quenches of the external field in the transverse field Ising chain have been considered in [Calabrese et al., 2012a,b], among other works. In [Calabrese et al., 2012b], the authors found that the system approaches a stationary state and that the stationary properties are, in fact, given by an appropriately defined generalized Gibbs ensemble. Moreover, in [Calabrese et al., 2012a], the time dependence of the longitudinal correlation function after a sudden quench for asymptotically large values of the time passed after the quench and for the relative separation of spins has been determined analytically for quenches within the ferromagnetic and within the paramagnetic phases.

The objective of this work is to analyse the dynamics of the transverse field Ising chain after a sudden quench. Our considerations are based on the results provided in [Calabrese et al., 2012a,b]. In particular, we are interested in the non-equlibrium dynamics after a sudden quench from a large intial value of the external field to the vicinity of the quantum critical point within the paramagnetic phase. We will investigate the longitudinal correlation function after a sudden quench and compare numerical calculations to the asymptotic expressions provided in the aforementioned works. Based on comparisons to our numerical calculations, we conjecture a refinement of a result given in [Calabrese et al., 2012a] for this correlation function. Our improved formula then implies that the behaviour of the correlator is characterized by two correlation lengths, one of which is the one obtained from a generalized Gibbs ensemble. Further, we also find that the correlator attains its stationary value rather quickly over short distances, which is an interesting observation with regard to experiments since it allows to detect stationary behaviour already at experimentally accessible regimes.

This work is organized as follows. In the first chapter, we will discuss in detail how to determine the spectrum of the transverse field Ising chain and examine the structure of the ground state of the model. In particular, we demonstrate see that the system exhibits a quantum phase transition in the thermodynamic limit. This detailed derivation is important as the solutions provided in the literature often assume simplifications and, thus, fail to correctly describe the system when these assumptions are dropped. In the second chapter, we consider the spin correlation functions with respect to the ground state of the transverse field Ising chain. In particular, we will examine the behaviour of the longitudinal correlator for large relative separations of the spins. These calculations will help us to understand the calculations of the longitudinal correlation function after a sudden quench of the transverse external field, which is treated in the third chapter. There, we will describe how to determine the longitudinal correlator and compare numerical calculations of this correlator with results provided in [Calabrese et al., 2012a]. Based on these comparisons, we conjecture an improved formula for the description of the time dependence of the longitudinal correlation function after a sudden quench.

2 The Spectrum of the Transverse Ising Chain

Let $\mathcal{H}$ be the Hilbert space of a single spin-1/2 system. That is, $\mathcal{H}$ is a two-dimensional complex linear space equipped with an inner product. Further, let I denote the identity and let X, Y, and Z be the Pauli operators on $\mathcal{H}$. Then, the Hilbert space of N such spin-1/2 systems, where N is a positive integer, is given by $\mathcal{H}_N \coloneqq \mathcal{H}^{\otimes N}$, and has the dimension 2^N. We can define Pauli operators on this Hilbert space of the composite system by

$$X_j \coloneqq I^{\otimes(j-1)} \otimes X \otimes I^{\otimes(N-j)}\,, \tag{2.1}$$

$$Y_j \coloneqq I^{\otimes(j-1)} \otimes Y \otimes I^{\otimes(N-j)}\,, \tag{2.2}$$

$$Z_j \coloneqq I^{\otimes(j-1)} \otimes Z \otimes I^{\otimes(N-j)}\,, \tag{2.3}$$

for all $j \in \{0, 1, \ldots, N-1\}$. We will interpret the compound system as a chain of N sites. Each of these sites constitutes a spin-1/2 system and is labeled by an index $j \in \{0, 1, \ldots, N-1\}$. The Hamiltonian given by

$$H = -g \sum_{j=0}^{N-1} X_j X_{j+1 \bmod N} - h \sum_{j=0}^{N-1} Z_j\,, \tag{2.4}$$

where g and h are non-zero real numbers, together with the Hilbert space $\mathcal{H}_N$, defines the Ising chain in a transverse field with periodic boundary conditions. We will refer to this model as the transverse Ising chain for short.

The Hamiltonian given by expression (2.4) consists of two parts, which are given by the two different sums. The first sum describes the interactions between the spins and corresponds to the Hamiltonian of the simple Ising model. The interactions are restricted to the nearest-neighbours and the coupling energy between the spins, g, is constant. The sign of the first part is chosen such that the system has ferromagnetic behaviour for positive values of g. The second part, that is, the second sum, describes a perturbation of the simple Ising chain by a transverse external field. The number h is an energy scale which is proportional to the field strength of the external field. Thus, we will call h simply the external field strength. The sign of this part is chosen such that the spins tend to align along the direction of the external field for increasing positive values of h.

A key feature of the transverse Ising chain is that the spectrum of the Hamiltonian has been constructed exactly. Shigetoshi Katsura determined the spectrum of the XY chain in a transverse field in [Katsura, 1962], of which the transverse Ising chain is a special case. Pierre Pfeuty later diagonalized the transverse Ising chain directly in [Pfeuty, 1970]. Both of them used a method employed by Elliott Lieb, Theodore Schultz, and Daniel Mattis to solve the simple XY chain without any external field by expressing the Hamiltonian of the model in terms of a particular set of fermionic operators, called the Jordan-Wigner operators [Lieb et al., 1961].

Another distinguishing property of the transverse Ising chain is that it is the simplest model to exhibit a quantum phase transition. A quantum phase transition is considered to be a phase transition at zero temperature and it takes place at a quantum critical point. A quantum critical point is, as defined in Subir Sachdev's book [Sachdev, 2011] on the subject, a point of non-analycity of the energy density of the ground state in the thermodynamic limit, $N \to \infty$. Since the spectrum of the transverse Ising chain can be constructed explicitly, the ground state energy density in the thermodynamic limit can be obtained straightforwardly and it is possible to pinpoint the quantum critical point.

The purpose of this chapter is to outline the diagonalization of the Hamiltonian (2.4) of the transverse Ising chain. We begin by expressing the Hamiltonian in terms of the fermionic Jordan-Wigner operators. This leads to the observation that the Hamiltonian of the system can be expressed as the orthogonal sum of two Hermitian operators. Each of these two operators will be diagonalized separately by performing a Fourier transformation, followed by the introduction of fermionic Bogoliubov operators. The eigenvalues and eigenvectors of the Hamiltonian can then be constructed from the eigenvalues and eigenvectors of these two operators. We will consider the ground state and the ground state energy of the transverse Ising chain in more detail. In particular, we will show that the system has a quantum critical point at $h = g$ in the thermodynamic limit.

2.1 Fermionization of the Hamiltonian

For all $j \in \{0, 1, \ldots, N-1\}$, we define the operators

$$\sigma_j \coloneqq \frac{1}{2}(X_j + \mathrm{i}Y_j)\,. \tag{2.5}$$

These are the spin-raising operators associated with each site of the circular chain. Their Hermitian conjugates,

$$\sigma_j^\dagger = \frac{1}{2}(X_j - \mathrm{i}Y_j)\,, \tag{2.6}$$

are the corresponding spin-lowering operators. We define the Jordan-Wigner operators, a_j, in terms of these raising and lowering operators by

$$a_j \coloneqq \exp\left(\mathrm{i}\pi \sum_{k=0}^{j-1} \sigma_k^\dagger \sigma_k\right) \sigma_j \,. \tag{2.7}$$

The Jordan-Wigner operators are fermionic which means that they satisfy the canonical anticommutation relations

$$a_j a_k + a_k a_j = 0 \,, \tag{2.8}$$

$$a_j a_k^\dagger + a_k^\dagger a_j = \delta_{jk} \,, \tag{2.9}$$

for all $j, k \in \{0, 1, \ldots, N-1\}$. A proof of this statement is given in the Appendix A.

Let $j \in \{0, 1, \ldots, N-1\}$. It follows immediately from the definition of the Jordan-Wigner operators that

$$a_j^\dagger a_j = \sigma_j^\dagger \sigma_j \,. \tag{2.10}$$

Using this last identity in conjunction with the definition of the Jordan-Wigner operators gives

$$\sigma_j = \exp\left(-\mathrm{i}\pi \sum_{k=0}^{j-1} a_k^\dagger a_k\right) a_j \,. \tag{2.11}$$

With this, we have expressed the spin-raising and, thus, also the spin-lowering operators solely in terms of the Jordan-Wigner operators.

For any $j \in \{0, 1, \ldots, N-1\}$, we have that

$$X_j = \sigma_j^\dagger + \sigma_j \,, \tag{2.12}$$

$$Y_j = \mathrm{i}\left(\sigma_j^\dagger - \sigma_j\right) \,, \tag{2.13}$$

$$Z_j = I - 2\sigma_j^\dagger \sigma_j \,. \tag{2.14}$$

The identities for X_j and Y_j follow directly by substituting the expressions for σ_j and $\sigma_j^\dagger$, which are given in (2.5) and (2.6). The last identity for Z_j is obtained by, additionally, using the commutation relation $X_j Y_j - Y_j X_j = 2\mathrm{i} Z_j$. These identities allow us to rewrite the Pauli operators in terms of the Jordan-Wigner operators by using (2.11), which, ultimately, allows us to express the Hamiltonian, H, solely in terms of the Jordan-Wigner operators.

Before we derive expressions for the Pauli operators in terms of the Jordan-Wigner operators, we analyse the operator

$$\exp\left(\mathrm{i}\pi \sum_{k=0}^{j-1} a_k^\dagger a_k\right) \,,$$

in more detail. It follows from the canonical anticommutation relations for the Jordan-Wigner operators, which are given in (2.8) and (2.9), that the operators $a_k^\dagger a_k$, $k \in \{0, 1, \ldots, N-1\}$, mutually commute. Therefore, we can factorize the expression

$$\exp\left(\mathrm{i}\pi \sum_{k=0}^{j-1} a_k^\dagger a_k\right) = \prod_{k=0}^{j-1} \exp\left(\mathrm{i}\pi a_k^\dagger a_k\right) \tag{2.15}$$

for all $j \in \{0, 1, \ldots, N-1\}$. This implies that it is sufficient to examine the operator $\exp\left(\mathrm{i}\pi a_j^\dagger a_j\right)$ for $j \in \{0, 1, \ldots, N-1\}$ in more detail.

At this point, it is convenient to introduce the Fock basis vectors of the Jordan-Wigner operators. These will be denoted by φ_n, where $n = (n_0, n_1, \ldots, n_{N-1}) \in \{0,1\}^N$, and they satisfy $a_j^\dagger a_j \varphi_n = n_j \varphi_n$ for any $j \in \{0, 1, \ldots, N-1\}$.

By considering the action of $\exp\left(\mathrm{i}\pi a_j^\dagger a_j\right)$ on a Fock basis vector φ_n for $n \in \{0,1\}^N$ and for $j \in \{0, 1, \ldots, N-1\}$, we obtain the identities

$$\exp\left(\mathrm{i}\pi a_j^\dagger a_j\right) = \exp\left(-\mathrm{i}\pi a_j^\dagger a_j\right) , \tag{2.16}$$

and

$$\exp\left(\mathrm{i}\pi a_j^\dagger a_j\right) = I - 2a_j^\dagger a_j . \tag{2.17}$$

Additionally, using the canonical anticommutation relations for the Jordan-Wigner operators given in (2.8) and (2.9), we obtain that

$$I - 2a_j^\dagger a_j = \left(a_j^\dagger + a_j\right)\left(a_j^\dagger - a_j\right) , \tag{2.18}$$

for all $j \in \{0, 1, \ldots, N-1\}$.

Let us now express the Pauli operators in terms of the fermionic Jordan-Wigner operators. Let $j \in \{0, 1, \ldots, N-1\}$. We begin with X_j, for which we can use the equations (2.11) and (2.12) to obtain that

$$X_j = a_j^\dagger \exp\left(\mathrm{i}\pi \sum_{k=0}^{j-1} a_k^\dagger a_k\right) + \exp\left(-\mathrm{i}\pi \sum_{k=0}^{j-1} a_k^\dagger a_k\right) a_j .$$

This expression can be further simplified by using (2.16) and by observing that a_k, as well as $a_k^\dagger$, commutes with $a_l^\dagger a_l$ if $k \neq l$. We obtain that

$$X_j = \exp\left(\mathrm{i}\pi \sum_{k=0}^{j-1} a_k^\dagger a_k\right)\left(a_j^\dagger + a_j\right) . \tag{2.19}$$

We can perform an analogous derivation for Y_j by starting from (2.11) and (2.13), which yields

$$Y_j = \mathrm{i}\exp\left(\mathrm{i}\pi \sum_{k=0}^{j-1} a_k^\dagger a_k\right)\left(a_j^\dagger - a_j\right) . \tag{2.20}$$

For Z_j, we use (2.10) and (2.14) to obtain that

$$Z_j = I - 2a_j^\dagger a_j \,. \tag{2.21}$$

In principle, we are in a position to express the Hamiltonian of the transverse Ising chain solely in terms of the fermionic Jordan-Wigner operators. We only need to substitute the expressions (2.19) and (2.21) into the expression (2.4) for the Hamiltonian. However, the Hamiltonian involves products of the Pauli operators X_j, which we consider separately.

For all $j \in \{0, 1, \ldots, N-1\}$, we define the operators

$$A_j \coloneqq a_j^\dagger + a_j \,, \tag{2.22}$$

$$B_j \coloneqq a_j^\dagger - a_j \,. \tag{2.23}$$

These operators satisfy the anticommutation relations

$$A_j A_k + A_k A_j = 2\delta_{jk} \,, \tag{2.24}$$

$$B_j B_k + B_k B_j = -2\delta_{jk} \,, \tag{2.25}$$

$$A_j B_k + B_k A_j = 0 \,, \tag{2.26}$$

for all $j, k \in \{0, 1, \ldots, N-1\}$. In particular, the anticommutation relations given in (2.24) and (2.25) imply that $A_j^2 = I$ and that $B_j^2 = -I$ for all $j \in \{0, 1, \ldots, N-1\}$. Furthermore, we can use (2.17) and (2.18) to write

$$\exp\left(\mathrm{i}\pi a_j^\dagger a_j\right) = A_j B_j \,, \tag{2.27}$$

for all $j \in \{0, 1, \ldots, N-1\}$.

Let $j \in \{0, 1, \ldots, N-2\}$. By using (2.19), we obtain that

$$X_j X_{j+1} = \left(a_j^\dagger + a_j\right) \exp\left(\mathrm{i}\pi a_j^\dagger a_j\right) \left(a_{j+1}^\dagger + a_{j+1}\right) \,.$$

Expressing this identity in terms of the operators A_j and B_j using (2.22) and (2.27), we obtain that

$$X_j X_{j+1} = A_j A_j B_j A_{j+1} = B_j A_{j+1} \,.$$

Rewritting this identity in terms of the Jordan-Wigner operators gives that

$$X_j X_{j+1} = \left(a_j^\dagger - a_j\right) \left(a_{j+1}^\dagger + a_{j+1}\right) \,. \tag{2.28}$$

It remains to determine $X_{N-1}X_0$. Again, using (2.19), we obtain that

$$X_{N-1} X_0 = \left(a_{N-1}^\dagger + a_{N-1}\right) \exp\left(\mathrm{i}\pi \sum_{k=0}^{N-2} a_k^\dagger a_k\right) \left(a_0^\dagger + a_0\right) \,.$$

This can be rewritten in terms of the operators A_j and B_j to give

$$\begin{aligned}
X_{N-1}X_0 &= A_{N-1}A_0B_0A_1B_1\cdots A_{N-2}B_{N-2}A_0 \\
&= -A_{N-1}B_0A_1B_1\cdots A_{N-2}B_{N-2} \\
&= B_0A_1B_1\cdots A_{N-2}B_{N-2}A_{N-1} \\
&= -B_0A_1B_1\cdots A_{N-2}B_{N-2}A_{N-1}B_{N-1}^2 \\
&= -B_{N-1}A_0A_0B_0A_1B_1\cdots A_{N-1}B_{N-1}\,.
\end{aligned}$$

Expressing this identity in terms of the Jordan-Wigner operators gives

$$X_{N-1}X_0 = -\left(a_{N-1}^\dagger - a_{N-1}\right)\left(a_0^\dagger + a_0\right)\exp\left(\mathrm{i}\pi\sum_{k=0}^{N-1}a_k^\dagger a_k\right)\,. \tag{2.29}$$

Finally, we are in a position to express the Hamiltonian, H, given in (2.4) solely in terms of the Jordan-Wigner operators. By using (2.21), (2.28), and (2.29), we obtain that

$$\begin{aligned}
H = \sum_{j=0}^{N-1}\left[2ha_j^\dagger a_j - g\left(a_j^\dagger - a_j\right)\left(a_{j+1 \bmod N}^\dagger + a_{j+1 \bmod N}\right)\right] - hN \\
+ g\left(a_{N-1}^\dagger - a_{N-1}\right)\left(a_0^\dagger + a_0\right)\left[I + \exp\left(\mathrm{i}\pi\sum_{k=0}^{N-1}a_k^\dagger a_k\right)\right]\,.
\end{aligned} \tag{2.30}$$

2.2 The Even and the Odd Subspaces

In this section, we will show by using (2.30) that the Hamiltonian, H, can be expressed as the direct sum of two mutually orthogonal Hermitian operators. Each of these operators will act on two subspaces of the Hilbert space, $\mathcal{H}_N$, which are given by orthogonal projections. This will allow us to reduce the diagonalization of the Hamiltonian of the transverse Ising chain to the diagonalization of two Hermitian operators which are quadratic in the Jordan-Wigner operators.

Let us introduce the operator

$$P \coloneqq \frac{1}{2}\left[I + \exp\left(\mathrm{i}\pi\sum_{j=0}^{N-1}a_j^\dagger a_j\right)\right]\,. \tag{2.31}$$

The operator P is Hermitian, $P = P^\dagger$, and idempotent, $P^2 = P$. Therefore, it is an orthogonal projection operator. The complementary projection operator is $Q \coloneqq I - P$, which can be explicitly written as

$$Q = \frac{1}{2}\left[I - \exp\left(\mathrm{i}\pi\sum_{j=0}^{N-1}a_j^\dagger a_j\right)\right]\,. \tag{2.32}$$

The Hilbert space of the compound system, $\mathcal{H}_N$, is the direct sum of the two orthogonal subspaces $P(\mathcal{H}_N)$ and $Q(\mathcal{H}_N)$. That is, we can write

$$\mathcal{H}_N = P(\mathcal{H}_N) \oplus Q(\mathcal{H}_N) \,. \tag{2.33}$$

We can use the Fock basis vectors, φ_n with $n \in \{0,1\}^N$, in order to characterize these two subspaces. Consider the action of P and Q on φ_n. When $|n| \coloneqq \sum_{j=0}^{N-1} |n_j|$, we find that

$$P\varphi_n = \frac{1}{2}\left(1 + e^{\mathrm{i}\pi|n|}\right)\varphi_n \,, \tag{2.34}$$

and

$$Q\varphi_n = \frac{1}{2}\left(1 - e^{\mathrm{i}\pi|n|}\right)\varphi_n \,. \tag{2.35}$$

Therefore, depending on whether the number $|n|$ is even or odd, we obtain that

$$P\varphi_n = \begin{cases} \varphi_n & \text{if } |n| \text{ is even,} \\ 0 & \text{otherwise,} \end{cases} \tag{2.36}$$

and

$$Q\varphi_n = \begin{cases} 0 & \text{if } |n| \text{ is even,} \\ \varphi_n & \text{otherwise.} \end{cases} \tag{2.37}$$

That is, we can characterize the two subspaces as

$$P(\mathcal{H}_N) = \operatorname{Span}\left\{\varphi_n \,\middle|\, n \in \{0,1\}^N \text{ and } |n| \text{ is even}\right\} \,, \tag{2.38}$$

and

$$Q(\mathcal{H}_N) = \operatorname{Span}\left\{\varphi_n \,\middle|\, n \in \{0,1\}^N \text{ and } |n| \text{ is odd}\right\} \,. \tag{2.39}$$

Accordingly, we will call $P(\mathcal{H}_N)$ the even subspace and $Q(\mathcal{H}_N)$ the odd subspace.

There is another, physically more illustrative, way of characterizing the even and the odd subspaces in terms of the eigenvectors of the Pauli operators Z_j. Let ζ_0 and ζ_1 in $\mathcal{H}$ be the two normalized eigenvectors of the Pauli operator Z, with respective eigenvalues $+1$ and -1. We will call the states represented by these two vectors the spin-up and the spin-down state, respectively. Since Z is Hermitian, these two vectors form an orthonormal basis of $\mathcal{H}$. Using these basis vectors, we can construct an orthonormal basis of $\mathcal{H}_N$ by setting

$$\chi_s \coloneqq \zeta_{s_0} \otimes \zeta_{s_1} \otimes \cdots \otimes \zeta_{s_{N-1}} \,, \tag{2.40}$$

for all $s \in \{0,1\}^N$. Since we also have

$$Z_j \chi_s = (-1)^{s_j} \chi_s \,, \tag{2.41}$$

for all $j \in \{0, 1, \ldots, N-1\}$, these vectors are also the eigenvectors of the Pauli operators Z_j with corresponding eigenvalues $(-1)^{s_j}$. Further, we can use (2.15), (2.17), and (2.21) to obtain that

$$\exp\left(\mathrm{i}\pi \sum_{j=0}^{N-1} a_j^\dagger a_j\right) = \prod_{j=0}^{N-1} Z_j \,, \tag{2.42}$$

which allows us to express the projection operators P and Q in terms of the Pauli operators Z_j. This implies that

$$P\chi_s = \frac{1}{2}\left(1 + (-1)^{|s|}\right)\chi_s \,, \tag{2.43}$$

and

$$Q\chi_s = \frac{1}{2}\left(1 - (-1)^{|s|}\right)\chi_s \,. \tag{2.44}$$

Thus, we obtain

$$P(\mathcal{H}_N) = \mathrm{Span}\left\{\chi_s \,\middle|\, s \in \{0,1\}^N \text{ and } |s| \text{ is even}\right\} \,, \tag{2.45}$$

and

$$Q(\mathcal{H}_N) = \mathrm{Span}\left\{\chi_s \,\middle|\, s \in \{0,1\}^N \text{ and } |s| \text{ is odd}\right\} \,. \tag{2.46}$$

The number $|s| = \sum_{j=0}^{N-1} |s_j|$ is the number of vectors representing the spin-down state in χ_s. Therefore, the even subspace, $P(\mathcal{H}_N)$, is spanned by all those basis vectors χ_s which represent an even number of spin-down states. Correspondingly, the odd subspace, $Q(\mathcal{H}_N)$, is spanned by all those basis vectors χ_s which represent an odd number of spin-down states.

Let us define on $\mathcal{H}_N$ the operators

$$\begin{aligned} H_P \coloneqq \sum_{j=0}^{N-1} \left[2h a_j^\dagger a_j - g\left(a_j^\dagger - a_j\right)\left(a_{j+1 \bmod N}^\dagger + a_{j+1 \bmod N}\right)\right] - hN \\ + 2g\left(a_{N-1}^\dagger - a_{N-1}\right)\left(a_0^\dagger + a_0\right) \,, \end{aligned} \tag{2.47}$$

and

$$H_Q \coloneqq \sum_{j=0}^{N-1} \left[2h a_j^\dagger a_j - g\left(a_j^\dagger - a_j\right)\left(a_{j+1 \bmod N}^\dagger + a_{j+1 \bmod N}\right)\right] - hN \,. \tag{2.48}$$

It follows from the canonical anticommutation relations given in (2.8) and (2.9) that H_P and H_Q are Hermitian operators. In addition, the expression (2.30) implies that $H\psi = H_P\psi$ for $\psi \in P(\mathcal{H}_N)$ and that $H\psi = H_Q\psi$ for $\psi \in Q(\mathcal{H}_N)$. Therefore, by using that $P + Q = I$, we obtain that

$$H\psi = H(P+Q)\psi = (HP + HQ)\psi = (H_P P + H_Q Q)\psi$$

for any $\psi \in \mathcal{H}_N$. That is, we have that

$$H = H_P P + H_Q Q \,. \tag{2.49}$$

The operators H_P and H_Q are quadratic in the fermionic Jordan-Wigner operators. Any operator which is quadratic in the Jordan-Wigner operators leaves the even and the odd subspace invariant. This can be seen by using the characterizations of both subspaces in terms of the Fock basis vectors. For any $j, k \in \{0, 1, \dots, N-1\}$, consider the action of any of the operators $a_j a_k$, $a_j^\dagger a_k^\dagger$, $a_j^\dagger a_k$, and $a_j a_k^\dagger$ on a Fock basis vector φ_n with some $n \in \{0,1\}^N$. The resulting vector is either zero or another Fock basis vector φ_m with an index $m \in \{0,1\}^N$ such that either $|m|$ and $|n|$ are equal or they differ by two. If the result is φ_m, then we see that $|m|$ and $|n|$ have the same parity.

Since H_P and H_Q leave $P(\mathcal{H}_N)$ and $Q(\mathcal{H}_N)$ invariant, they commute with P and Q. Therefore, the operators $H_P P$ and $H_Q Q$ are Hermitian and mutually orthogonal. Thus, we decomposed the Hamiltonian of the transverse Ising chain, H, into a direct sum of two mutually orthogonal Hermitian operators as can be seen in (2.49). As an immediate consequence, $H_P P$ on $P(\mathcal{H}_N)$ and $H_Q Q$ on $Q(\mathcal{H}_N)$ can be diagonalized separately in order to diagonalize H.

If $\psi \in \mathcal{H}_N$ is an eigenvector of H_P with the corresponding eigenvalue λ and if $P\psi \neq 0$, then $P\psi$ is an eigenvector of $H_P P$ with the same eigenvalue λ since H_P and P commute. Analogously, if $\psi \in \mathcal{H}_N$ is an eigenvector of H_Q with the corresponding eigenvalue λ and if $Q\psi \neq 0$, then $Q\psi$ is an eigenvector of $H_Q Q$ with the same eigenvalue λ since H_Q and Q commute. Therefore, it is sufficient to diagonalize H_P and H_Q on $\mathcal{H}_N$ and, then, construct a basis of $P(\mathcal{H}_N)$ of those eigenvectors of H_P which have a non-zero projection onto $P(\mathcal{H}_N)$, and construct a basis of $Q(\mathcal{H}_N)$ of those eigenvectors of H_Q which have a non-zero projection onto $Q(\mathcal{H}_N)$.

2.3 The Discrete Fourier Transformation

The first step towards the diagonalization of the operators H_P and H_Q is the introduction of momentum degrees of freedom for the Jordan-Wigner fermions. To this end, we introduce the discrete Fourier transforms of the Jordan-Wigner operators. Namely, for all $p \in \frac{\pi}{N}\mathbb{Z}$, define

$$b_p := \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} a_j e^{-\mathrm{i}pj} \,. \tag{2.50}$$

These operators have periodicity 2π, which means that $b_{p+2\pi} = b_p$ for all $p \in \frac{\pi}{N}\mathbb{Z}$. Further, the Fourier transforms satisfy canonical anticommutation relations in the following sense: for all $p, q \in \frac{\pi}{N}\mathbb{Z}$, we have that

$$b_p b_q + b_q b_p = 0\,, \tag{2.51}$$

$$b_p b_q^\dagger + b_q^\dagger b_p = \delta_{p-q=0 \bmod 2\pi}\,. \tag{2.52}$$

Note that if A denotes a condition, then δ_A will denote the indicator function of that condition, which is given by

$$\delta_A = \begin{cases} 1 & \text{if the condition } A \text{ is true,} \\ 0 & \text{otherwise.} \end{cases}$$

Our aim is to express H_P and H_Q in terms of these Fourier transformed operators.

Let us first consider H_P. We introduce the set

$$P_N := \begin{cases} \frac{2\pi}{N}\left\{-\frac{N-1}{2}, -\frac{N-3}{2}, \dots, \frac{N-1}{2}\right\} & \text{if } N \text{ is even,} \\ \frac{2\pi}{N}\left\{-\frac{N}{2}, -\frac{N}{2}+1, \dots, \frac{N}{2}-1\right\} & \text{if } N \text{ is odd.} \end{cases} \tag{2.53}$$

For all $j \in \mathbb{Z}$, we define

$$\tilde{a}_j := \frac{1}{\sqrt{N}} \sum_{p \in P_N} b_p e^{\mathrm{i}pj}\,. \tag{2.54}$$

These operators satisfy $\tilde{a}_{j+N} = -\tilde{a}_j$ for all $j \in \mathbb{Z}$, which means that they are antiperiodic. Furthermore, for all $j \in \{0, 1, \dots, N-1\}$, we have that $\tilde{a}_j = a_j$. Therefore, the operators $\tilde{a}_j$ are the antiperiodic extension of the fermionic Jordan-Wigner operators to all integers. This, in turn, allows us to rewrite the operator H_P in the form

$$H_P = \sum_{j=0}^{N-1} \left[2h\tilde{a}_j^\dagger \tilde{a}_j - g\left(\tilde{a}_j^\dagger - \tilde{a}_j\right)\left(\tilde{a}_{j+1}^\dagger + \tilde{a}_{j+1}\right)\right] - hN\,. \tag{2.55}$$

Substituting the definitions of the operators $\tilde{a}_j$ in terms of the Fourier transforms and simplifying the resulting expression, the operator H_P takes the form

$$H_P = \sum_{p \in P_N} \left[2(h - g\cos p)\left(b_p^\dagger b_p - \frac{1}{2}\right) - g e^{\mathrm{i}p} b_p^\dagger b_{-p}^\dagger + g e^{-\mathrm{i}p} b_p b_{-p}\right]. \tag{2.56}$$

The last expression for H_P can be further simplified. To this end, we need to differentiate between the cases where N is even and where N is odd. We start by assuming that N is even. Then, the set over which the summation in (2.56) is taken contains pairs of positive and corresponding negative values, namely

$$\pm\frac{2\pi}{N}\frac{1}{2}, \pm\frac{2\pi}{N}\frac{3}{2}, \dots, \pm\frac{2\pi}{N}\frac{N-1}{2}\,.$$

This allows us to split the sum into two parts, one in which we take the sum over the positive summation indices and one in which we take the sum over the corresponding negative summation indices. Subsequently, we rewrite the sum over the negative summation indices in terms of the positive summation indices and combine the terms. Using matrices, the resulting expression reads

$$H_P = \sum_{p \in P_N^+} \begin{bmatrix} b_p^\dagger & b_{-p} \end{bmatrix} \begin{bmatrix} 2(h - g\cos p) & -2\mathrm{i}g\sin p \\ 2\mathrm{i}g\sin p & -2(h - g\cos p) \end{bmatrix} \begin{bmatrix} b_p \\ b_{-p}^\dagger \end{bmatrix} , \tag{2.57}$$

where P_N^+ is the set of the positive elements in P_N.

Now, assume that N is odd. Again, the set over which the summation in (2.56) is performed contains pairs of positive and corresponding negative values, namely

$$\pm\frac{2\pi}{N}\frac{1}{2}, \pm\frac{2\pi}{N}\frac{3}{2}, \ldots, \pm\frac{2\pi}{N}\left(\frac{N}{2} - 1\right) ,$$

but, in contrast to the even N case, there is no corresponding positive number for $-\pi$ in P_N. Again, splitting the sum into a sum over negative and a sum over positive summation indices, rewriting the negative summation indices in terms of positive ones where possible, and combining terms, we obtain

$$\begin{aligned} H_P = {} & 2(h + g)\left(b_{-\pi}^\dagger b_{-\pi} - \frac{1}{2}\right) \\ & + \sum_{p \in P_N^+} \begin{bmatrix} b_p^\dagger & b_{-p} \end{bmatrix} \begin{bmatrix} 2(h - g\cos p) & -2\mathrm{i}g\sin p \\ 2\mathrm{i}g\sin p & -2(h - g\cos p) \end{bmatrix} \begin{bmatrix} b_p \\ b_{-p}^\dagger \end{bmatrix} . \end{aligned} \tag{2.58}$$

Next, we consider the operator H_Q. We introduce the set

$$Q_N := \begin{cases} \frac{2\pi}{N}\left\{-\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1\right\} & \text{if } N \text{ is even,} \\ \frac{2\pi}{N}\left\{-\frac{N-1}{2}, -\frac{N-3}{2}, \ldots, \frac{N-1}{2}\right\} & \text{if } N \text{ is odd.} \end{cases} \tag{2.59}$$

For all $j \in \mathbb{Z}$, we define

$$\hat{a}_j := \frac{1}{\sqrt{N}} \sum_{p \in Q_N} b_p e^{\mathrm{i}pj} . \tag{2.60}$$

These operators satisfy $\hat{a}_{j+N} = \hat{a}_j$ for all $j \in \mathbb{Z}$, which means that they are periodic. Furthermore, for all $j \in \{0, 1, \ldots, N - 1\}$, we have $\hat{a}_j = a_j$. Therefore, the operators $\hat{a}_j$ are the periodic extension of the fermionic Jordan-Wigner operators to all integers. This, in turn, allows us to rewrite the operator H_Q in the form

$$H_Q = \sum_{j=0}^{N-1} \left[2h\hat{a}_j^\dagger \hat{a}_j - g\left(\hat{a}_j^\dagger - \hat{a}_j\right)\left(\hat{a}_{j+1}^\dagger + \hat{a}_{j+1}\right)\right] - hN . \tag{2.61}$$

Substituting the definitions of the operators $\hat{a}_j$ in terms of the Fourier transforms gives that

$$H_Q = \sum_{p\in Q_N} \left[2(h - g\cos p)\left(b_p^\dagger b_p - \frac{1}{2}\right) - ge^{\mathrm{i}p} b_p^\dagger b_{-p}^\dagger + ge^{-\mathrm{i}p} b_p b_{-p}\right] . \tag{2.62}$$

In complete analogy to our calculations for H_P, introducing the set Q_N^+ of positive elements in Q_N and differentiating between the cases where N is even and where N is odd, we obtain that

$$\begin{aligned} H_Q = {} & 2(h+g)\left(b_{-\pi}^\dagger b_{-\pi} - \frac{1}{2}\right) + 2(h-g)\left(b_0^\dagger b_0 - \frac{1}{2}\right) \\ & + \sum_{p\in Q_N^+} \begin{bmatrix} b_p^\dagger & b_{-p} \end{bmatrix} \begin{bmatrix} 2(h-g\cos p) & -2\mathrm{i}g\sin p \\ 2\mathrm{i}g\sin p & -2(h-g\cos p) \end{bmatrix} \begin{bmatrix} b_p \\ b_{-p}^\dagger \end{bmatrix} , \end{aligned} \tag{2.63}$$

if N is even and

$$\begin{aligned} H_Q = {} & 2(h-g)\left(b_0^\dagger b_0 - \frac{1}{2}\right) \\ & + \sum_{p\in Q_N^+} \begin{bmatrix} b_p^\dagger & b_{-p} \end{bmatrix} \begin{bmatrix} 2(h-g\cos p) & -2\mathrm{i}g\sin p \\ 2\mathrm{i}g\sin p & -2(h-g\cos p) \end{bmatrix} \begin{bmatrix} b_p \\ b_{-p}^\dagger \end{bmatrix} , \end{aligned} \tag{2.64}$$

if N is odd.

2.4 The Bogoliubov Transformation

In the preceding section, we expressed H_P and H_Q in terms of Fourier tranformed Jordan-Wigner operators. The resulting expressions for H_P are given in (2.57) and (2.58), and the ones for H_Q are given in (2.63) and (2.64). In any case, we can assign the terms in these equations to one of the following three types. The first one is

$$S_1(p) \coloneqq 2(h-g)\left(b_p^\dagger b_p - \frac{1}{2}\right) , \tag{2.65}$$

where $p \in 2\pi\mathbb{Z}$. The second type is

$$S_2(p) \coloneqq 2(h+g)\left(b_p^\dagger b_p - \frac{1}{2}\right) , \tag{2.66}$$

where $p \in 2\pi\left(\mathbb{Z} + \frac{1}{2}\right)$. The third and last type is given by

$$S_3(p) \coloneqq \begin{bmatrix} b_p^\dagger & b_{-p} \end{bmatrix} \begin{bmatrix} 2(h-g\cos p) & -2\mathrm{i}g\sin p \\ 2\mathrm{i}g\sin p & -2(h-g\cos p) \end{bmatrix} \begin{bmatrix} b_p \\ b_{-p}^\dagger \end{bmatrix} , \tag{2.67}$$

where $p \in \frac{\pi}{N}\mathbb{Z}$ but $p \notin \pi\mathbb{Z}$.

Let us start by considering the third type involving the matrix. The matrix in (2.67) is Hermitian and, thus, can be diagonalized by a unitary transformation. This unitary matrix is not unique and it will transform the Fourier transforms of the Jordan-Wigner operators accordingly. By choosing the unitary matrix appropriately, we will obtain a new kind of fermions in terms of which $S_3(p)$ will become diagonal.

We consider a more general matrix than given in (2.67). Namely, we will allow p to be real-valued. To this end, for all $p \in \mathbb{R}$, let

$$\alpha_p := 2(h - g\cos p)\,, \tag{2.68}$$

$$\beta_p := -2\mathrm{i}g\sin p\,, \tag{2.69}$$

and let M_p be the two by two matrix given by

$$M_p := \begin{bmatrix} \alpha_p & \beta_p \\ -\beta_p & -\alpha_p \end{bmatrix}\,. \tag{2.70}$$

For all $p \in \mathbb{R}$, the matrix M_p is Hermitian and, thus, it can be diagonalized. The characteristic equation for the eigenvalues λ of M_p reads

$$\lambda^2 - |\alpha_p|^2 - |\beta_p|^2 = 0\,.$$

The solutions are given by $\lambda = \omega_p$ and $\lambda = -\omega_p$, where

$$\omega_p := 2\sqrt{g^2 + h^2 - 2gh\cos p}\,. \tag{2.71}$$

We note that the matrix M_p is already diagonal for all $p \in \pi\mathbb{Z}$ since, for such p, we have that $\beta_p = 0$. However, the terms of third type do not involve any such p. Thus, we can restrict our considerations to the case where $p \in \mathbb{R}$ but $p \notin \pi\mathbb{Z}$.

Let $p \in \mathbb{R}$ with $p \notin \pi\mathbb{Z}$. Then, we have that $\omega_p \neq -\omega_p$. Since M_p is Hermitian, this means that the eigenspaces of M_p for the eigenvalues ω_p and $-\omega_p$ are one-dimensional and mutually orthogonal.

The structure of M_p allows us to make statements about the eigenvectors without explicitly determining them. For any $p \in \mathbb{R}$ with $p \notin \pi\mathbb{Z}$, let $[u_p^* \;\; v_p^*]^{\mathrm{T}}$ denote a normalized eigenvector of M_p with the corresponding eigenvalue ω_p. That is, we have that $|u_p|^2 + |v_p|^2 = 1$ and

$$\omega_p \begin{bmatrix} u_p^* \\ v_p^* \end{bmatrix} = \begin{bmatrix} \alpha_p & \beta_p \\ -\beta_p & -\alpha_p \end{bmatrix} \begin{bmatrix} u_p^* \\ v_p^* \end{bmatrix} = \begin{bmatrix} \alpha_p u_p^* + \beta_p v_p^* \\ -\beta_p u_p^* - \alpha_p v_p^* \end{bmatrix}\,. \tag{2.72}$$

In particular, since M_p is 2π-periodic, we can choose u_p and v_p such that they are 2π-periodic, too. Equation (2.72) implies that $[v_p^* \;\; u_p^*]^{\mathrm{T}}$ is a normalized eigenvector of M_p with the eigenvalue $-\omega_p$ since

$$\begin{bmatrix} \alpha_p & \beta_p \\ -\beta_p & -\alpha_p \end{bmatrix} \begin{bmatrix} v_p^* \\ u_p^* \end{bmatrix} = \begin{bmatrix} \alpha_p v_p^* + \beta_p u_p^* \\ -\beta_p v_p^* - \alpha_p u_p^* \end{bmatrix} = -\omega_p \begin{bmatrix} v_p^* \\ u_p^* \end{bmatrix} . \tag{2.73}$$

Additionally, since the eigenspaces of M_p are mutually orthogonal for $p \in \mathbb{R}$ with $p \notin \pi\mathbb{Z}$, we have that $[u_p^* \;\; v_p^*]^{\mathrm{T}}$ and $[v_p^* \;\; u_p^*]^{\mathrm{T}}$ are mutually orthogonal. That is, we have that $u_p v_p^* + v_p u_p^* = 0$.

For $p \in \mathbb{R}$ with $p \notin \pi\mathbb{Z}$, consider the eigenvalue equation

$$\begin{bmatrix} \alpha_p & \beta_p \\ -\beta_p & -\alpha_p \end{bmatrix} \begin{bmatrix} u_p^* \\ v_p^* \end{bmatrix} = \omega_p \begin{bmatrix} u_p^* \\ v_p^* \end{bmatrix}$$

once again. Taking the complex conjugate of both sides of the equation and using that $\alpha_p = \alpha_{-p} = \alpha_p^*$, $\beta_p = -\beta_{-p} = -\beta_p^*$, and $\omega_p = \omega_{-p} = \omega_p^*$, we obtain that

$$\begin{bmatrix} \alpha_{-p} & \beta_{-p} \\ -\beta_{-p} & -\alpha_{-p} \end{bmatrix} \begin{bmatrix} u_p \\ v_p \end{bmatrix} = \omega_{-p} \begin{bmatrix} u_p \\ v_p \end{bmatrix} .$$

This is the eigenvalue equation of M_{-p} for the eigenvalue ω_{-p}. Since the corresponding eigenspace is one-dimensional and since $[u_p \;\; v_p]^{\mathrm{T}}$ and $[u_{-p}^* \;\; v_{-p}^*]^{\mathrm{T}}$ are normalized to one, we obtain that $[u_p \;\; v_p]^{\mathrm{T}}$ and $[u_{-p}^* \;\; v_{-p}^*]^{\mathrm{T}}$ can only differ by a complex factor of modulus one. This means that there is a $\phi_p \in [-\pi, \pi[$ such that $u_p = e^{\mathrm{i}\phi_p} u_{-p}^*$ and $v_p = e^{\mathrm{i}\phi_p} v_{-p}^*$. Therefore, the identity $u_p v_p^* + v_p u_p^* = 0$ can be cast into the form $u_p v_{-p} + v_p u_{-p} = 0$.

For $p \in \mathbb{R}$ with $p \notin \pi\mathbb{Z}$, we choose

$$u_p := \frac{\alpha_p + \omega_p}{\sqrt{2\omega_p(\alpha_p + \omega_p)}} , \tag{2.74}$$

$$v_p := \frac{\beta_p}{\sqrt{2\omega_p(\alpha_p + \omega_p)}} . \tag{2.75}$$

This choice is special since we have that $u_p = u_{-p}^*$ and $v_p = v_{-p}^*$ for this particular choice. For the expression (2.67), we obtain that

$$\begin{aligned} &\begin{bmatrix} b_p^\dagger & b_{-p} \end{bmatrix} \begin{bmatrix} \alpha_p & \beta_p \\ -\beta_p & -\alpha_p \end{bmatrix} \begin{bmatrix} b_p \\ b_{-p}^\dagger \end{bmatrix} \\ &\quad = \begin{bmatrix} b_p^\dagger & b_{-p} \end{bmatrix} \begin{bmatrix} u_p^* & v_p^* \\ v_p^* & u_p^* \end{bmatrix} \begin{bmatrix} u_p & v_p \\ v_p & u_p \end{bmatrix} \begin{bmatrix} \alpha_p & \beta_p \\ -\beta_p & -\alpha_p \end{bmatrix} \begin{bmatrix} u_p^* & v_p^* \\ v_p^* & u_p^* \end{bmatrix} \begin{bmatrix} u_p & v_p \\ v_p & u_p \end{bmatrix} \begin{bmatrix} b_p \\ b_{-p}^\dagger \end{bmatrix} . \end{aligned}$$

We have that

$$\begin{bmatrix} u_p & v_p \\ v_p & u_p \end{bmatrix} \begin{bmatrix} \alpha_p & \beta_p \\ -\beta_p & -\alpha_p \end{bmatrix} \begin{bmatrix} u_p^* & v_p^* \\ v_p^* & u_p^* \end{bmatrix} = \begin{bmatrix} \omega_p & 0 \\ 0 & -\omega_p \end{bmatrix} ,$$

and that

$$\begin{bmatrix} u_p & v_p \\ v_p & u_p \end{bmatrix} \begin{bmatrix} b_p \\ b_{-p}^\dagger \end{bmatrix} = \begin{bmatrix} u_p b_p + v_p b_{-p}^\dagger \\ v_p b_p + u_p b_{-p}^\dagger \end{bmatrix} \tag{2.76}$$

We introduce the operators

$$c_p := u_p b_p + v_p b_{-p}^\dagger ,$$

where $p \in \frac{\pi}{N}\mathbb{Z}$ with $p \notin \pi\mathbb{Z}$. Since $u_p = u_{-p}^*$ and $v_p = v_{-p}^*$, we have that

$$v_p b_p + u_p b_{-p}^\dagger = v_{-p}^* b_p + u_{-p}^* b_{-p}^\dagger = c_{-p}^\dagger .$$

Therefore, we obtain for $S_3(p)$ the following result

$$S_3(p) = \begin{bmatrix} b_p^\dagger & b_{-p} \end{bmatrix} \begin{bmatrix} \alpha_p & \beta_p \\ -\beta_p & -\alpha_p \end{bmatrix} \begin{bmatrix} b_p \\ b_{-p}^\dagger \end{bmatrix} = \omega_p \left(c_p^\dagger c_p - c_{-p} c_{-p}^\dagger \right) .$$

It remains to consider the expressions (2.65) and (2.66). We study the expression (2.65) first. This operator has already the form of a fermionic quantum harmonic oscillator. However, the corresponding dispersion $2(h-g)$ can be negative. In order to make sure that the dispersion is always positive, we set for all $p \in 2\pi\mathbb{Z}$, $c_p := b_p$ if $h - g \geq 0$ and $c_p := -\mathrm{i} b_{-p}^\dagger = -\mathrm{i} b_p^\dagger$ otherwise. Then, the expression (2.65) takes the form

$$S_1(p) = 2(h-g)\left(b_p^\dagger b_p - \frac{1}{2} \right) = \omega_p \left(c_p^\dagger c_p - \frac{1}{2} \right)$$

for all $p \in 2\pi\mathbb{Z}$. We treat the expression (2.66) in the same manner and set, for all $p \in 2\pi\left(\mathbb{Z} + \frac{1}{2}\right)$, $c_p := b_p$ if $h + g \geq 0$ and $c_p := -\mathrm{i} b_{-p}^\dagger = -\mathrm{i} b_p^\dagger$ otherwise. Then, the expression (2.66) takes the form

$$S_2(p) = 2(h+g)\left(b_p^\dagger b_p - \frac{1}{2} \right) = \omega_p \left(c_p^\dagger c_p - \frac{1}{2} \right)$$

for all $p \in 2\pi\left(\mathbb{Z} + \frac{1}{2}\right)$.

To unify the notation, we define

$$u_p := \begin{cases} 1 & \text{if } g \leq h, \\ 0 & \text{otherwise,} \end{cases} \tag{2.77}$$

$$v_p := \begin{cases} 0 & \text{if } g \leq h, \\ -\mathrm{i} & \text{otherwise} \end{cases} \tag{2.78}$$

for all $p \in 2\pi\mathbb{Z}$ and

$$u_p \coloneqq \begin{cases} 1 & \text{if } g \geq -h, \\ 0 & \text{otherwise,} \end{cases} \tag{2.79}$$

$$v_p \coloneqq \begin{cases} 0 & \text{if } g \geq -h, \\ -\mathrm{i} & \text{otherwise} \end{cases} \tag{2.80}$$

for all $p \in 2\pi\left(\mathbb{Z} + \frac{1}{2}\right)$. Then, we have that

$$c_p = u_p b_p + v_p b_{-p}^\dagger \tag{2.81}$$

for all $p \in \frac{\pi}{N}\mathbb{Z}$. The identities $|u_p|^2 + |v_p|^2 = 1$ and $u_p v_{-p} + v_p u_{-p} = 0$ imply that these operators satisfy the canonical anticommutation relations

$$c_p c_q + c_q c_p = 0\,, \tag{2.82}$$

$$c_p c_q^\dagger + c_q^\dagger c_p = \delta_{p-q=0 \bmod 2\pi}\,, \tag{2.83}$$

for all $p, q \in \frac{\pi}{N}\mathbb{Z}$, meaning that the operators are fermionic. They are called the Bogoliubov transformed operators. We will call them Bogoliubov operators for short.

Rewriting the expressions (2.65), (2.66), and (2.67) in terms of these Bogoliubov operators, we obtain

$$H_P = \sum_{p \in P_N} \omega_p \left(c_p^\dagger c_p - \frac{1}{2}\right)\,, \tag{2.84}$$

and

$$H_Q = \sum_{p \in Q_N} \omega_p \left(c_p^\dagger c_p - \frac{1}{2}\right)\,. \tag{2.85}$$

That is, H_P and H_Q take the form of fermionic harmonic oscillators and the eigenstates of these two operators are the corresponding Fock states of the Bogoliubov fermions, which can be considered as the elementary excitations of the system and are identified with fermionic quasiparticles. The function ω_p gives the dispersion of the Bogoliubov fermions, examples of which are shown in Figure 2.1 for different parameter choices h/g.

2.5 The Ground State and the Quantum Critical Point

In this section, we derive expressions for the ground states of the Hamiltonians H_P and H_Q in terms of the vacuum state of the Jordan-Wigner operators. We will then

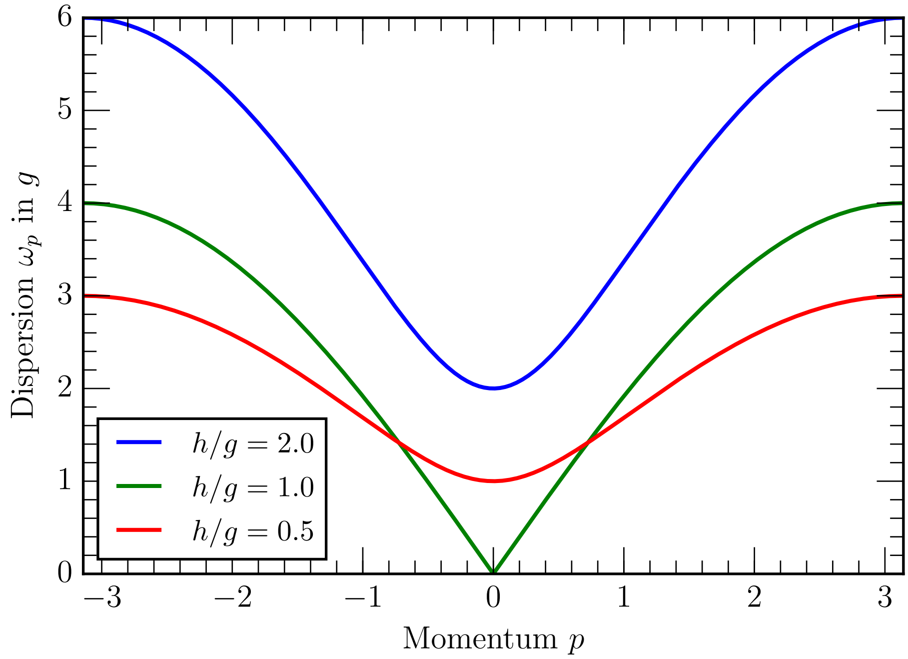

Figure 2.1: The dispersion of the Bogoliubov fermions in units of g. The dispersion is depicted for three different ratios of h/g. The dispersion has a gap at $p = 0$, which vanishes for $h/g = 1$. This indicates that there is a change in the system at $h/g = 1$.

construct the ground state of the Hamiltonian of the transverse Ising chain, H, using these expressions for the ground states of H_P and H_Q. This will allow us to make statements on the structure of the ground state and, in particular, find that, in the thermodynamic limit, there is a spontaneous symmetry breaking. We will also determine the ground state energy density in the thermodynamic limit and identify the quantum critical point at which a quantum phase transition occurs.

Since the dispersion of the Bogoliubov fermions, ω_p, is non-negative, Equations (2.84) and (2.85) imply that the ground states of H_P and H_Q are the vacuum states of the fermionic Bogoliubov operators c_p for $p \in P_N$ and $p \in Q_N$, respectively.

The vacuum state of the Jordan-Wigner operators is also the vacuum state of their Fourier transforms. This statement follows directly from the definition of the Fourier transforms in (2.50). Furthermore, from the inversions of the Fourier transforms given in (2.54) and (2.60), it follows that

$$\sum_{j=0}^{N-1} a_j^\dagger a_j = \sum_{p \in P_N} b_p^\dagger b_p = \sum_{p \in Q_N} b_p^\dagger b_p \,,$$

which, in turn, implies that

$$P = \frac{1}{2}\left[I + \exp\left(\mathrm{i}\pi \sum_{p \in P_N} b_p^\dagger b_p\right)\right] = \frac{1}{2}\left[I + \exp\left(\mathrm{i}\pi \sum_{p \in Q_N} b_p^\dagger b_p\right)\right] .$$

Therefore, the subspaces $P(\mathcal{H}_N)$ and $Q(\mathcal{H}_N)$ can be characterized by the Fock states of the Fourier transformed Jordan-Wigner operators in the same manner as we did characterize them in Section 2.2 using the Fock states of the Jordan-Wigner operators.

First, consider the ground state of H_P, represented by the normalized vector $\tilde{\Omega}$. We differentiate between the cases where N is even and where N is odd.

Let N be even. Then, we have that

$$\tilde{\Omega} \propto \left[\prod_{p \in P_N^+} c_p c_{-p}\right] \varphi_0 \,, \tag{2.86}$$

where φ_0 represents the vacuum of the Jordan-Wigner operators. We will keep overall normalization constants unspecified. That the right hand side represents, in fact, the ground state of H_P can be seen as follows. The canonical anticommutation relations for the Bogoliubov operators, which are given in (2.82) and (2.83), imply that

$$c_p \left[\prod_{q \in P_N^+} c_q c_{-q}\right] \varphi_0 = 0$$

for all $p \in P_N$. This is because we can anticommute c_p as long as $q \neq p$ and when $q = p$, and there is exactly one such q in the product, we obtain the above identity due to $c_p^2 = 0$. Furthermore, we can rewrite the right hand side of (2.86) as

$$\left[\prod_{p\in P_N^+} c_p c_{-p}\right]\varphi_0 \propto \left[\prod_{p\in P_N^+}\left(1-\frac{v_p}{u_p}b_p^\dagger b_{-p}^\dagger\right)\right]\varphi_0 = \exp\left(-\sum_{p\in P_N^+}\frac{v_p}{u_p}b_p^\dagger b_{-p}^\dagger\right)\varphi_0$$

Thus, the right hand side is non-zero and, alltogether, it represents the vacuum state of c_p for $p \in P_N$, which is also the ground state of H_P. So, we have that

$$\tilde{\Omega} \propto \exp\left(-\sum_{p\in P_N^+}\frac{v_p}{u_p}b_p^\dagger b_{-p}^\dagger\right)\varphi_0\,. \tag{2.87}$$

Since this expression involves only quadratic operators in $b_p^\dagger$, it follows that $\tilde{\Omega}$ is in the even subspace, that is,

$$P\tilde{\Omega} = \tilde{\Omega}\,. \tag{2.88}$$

For N being odd, there is the mode $p = -\pi$ in P_N which we need to treat separately since there is no corresponding positive value in P_N. All other modes come in positive and corresponding negative pairs and, thus, can be treated as in the even N case. The Bogoliubov operator $c_{-\pi}$ depends on the relation between g and h, as can be seen using (2.79), (2.80), and (2.81). If $g \geq -h$, we have that $c_{-\pi} = b_{-\pi}$ and, therefore, we can take

$$\tilde{\Omega} \propto \exp\left(-\sum_{p\in P_N^+}\frac{v_p}{u_p}b_p^\dagger b_{-p}^\dagger\right)\varphi_0$$

since $b_{-\pi}$ anticommutes with all the operators in this expression and annihilates the Jordan-Wigner vacuum. If, however, $g < -h$, then $c_{-\pi} = -\mathrm{i}b_{-\pi}^\dagger$ and we can take

$$\tilde{\Omega} \propto b_{-\pi}^\dagger \exp\left(-\sum_{p\in P_N^+}\frac{v_p}{u_p}b_p^\dagger b_{-p}^\dagger\right)\varphi_0$$

since $\left(b_{-\pi}^\dagger\right)^2 = 0$. In summary, we can represent the ground state of H_P by

$$\tilde{\Omega} \propto \begin{cases} \exp\left(-\sum_{p\in P_N^+}\frac{v_p}{u_p}b_p^\dagger b_{-p}^\dagger\right)\varphi_0 & \text{if } g \geq -h,\\ b_{-\pi}^\dagger \exp\left(-\sum_{p\in P_N^+}\frac{v_p}{u_p}b_p^\dagger b_{-p}^\dagger\right)\varphi_0 & \text{otherwise,}\end{cases} \tag{2.89}$$

where we again leave normalization factors unspecified. We have that

$$P\tilde{\Omega} = \begin{cases}\tilde{\Omega} & \text{if } g \geq -h,\\ 0 & \text{otherwise.}\end{cases} \tag{2.90}$$

Irrespective of whether N is even or odd, the energy of the ground state of the Hamiltonian H_P is

$$E_0^{(P)} = -\frac{1}{2}\sum_{p\in P_N} \omega_p\,. \tag{2.91}$$

Let us now consider the ground state of the Hamiltonian H_Q. For even N, the ground state is represented by

$$\hat{\Omega} \propto \begin{cases} \exp\Bigl(-\sum_{p\in Q_N^+} \frac{v_p}{u_p} b_p^\dagger b_{-p}^\dagger\Bigr)\varphi_0 & \text{if } g \le h \text{ and } g \ge -h,\\ b_0^\dagger \exp\Bigl(-\sum_{p\in Q_N^+} \frac{v_p}{u_p} b_p^\dagger b_{-p}^\dagger\Bigr)\varphi_0 & \text{if } g > h \text{ and } g \ge -h,\\ b_{-\pi}^\dagger \exp\Bigl(-\sum_{p\in Q_N^+} \frac{v_p}{u_p} b_p^\dagger b_{-p}^\dagger\Bigr)\varphi_0 & \text{if } g \le h \text{ and } g < -h,\\ b_{-\pi}^\dagger b_0^\dagger \exp\Bigl(-\sum_{p\in Q_N^+} \frac{v_p}{u_p} b_p^\dagger b_{-p}^\dagger\Bigr)\varphi_0 & \text{if } g > h \text{ and } g < -h. \end{cases} \tag{2.92}$$

The projection of this vector onto the odd subspace gives

$$Q\hat{\Omega} = \begin{cases} 0 & \text{if } g \le h \text{ and } g \ge -h,\\ \hat{\Omega} & \text{if } g > h \text{ and } g \ge -h,\\ \hat{\Omega} & \text{if } g \le h \text{ and } g < -h,\\ 0 & \text{if } g > h \text{ and } g < -h. \end{cases} \tag{2.93}$$

Similarly, for odd N, the ground state of H_Q is given by

$$\hat{\Omega} \propto \begin{cases} \exp\Bigl(-\sum_{p\in Q_N^+} \frac{v_p}{u_p} b_p^\dagger b_{-p}^\dagger\Bigr)\varphi_0 & \text{if } g \le h,\\ b_0^\dagger \exp\Bigl(-\sum_{p\in Q_N^+} \frac{v_p}{u_p} b_p^\dagger b_{-p}^\dagger\Bigr)\varphi_0 & \text{otherwise,} \end{cases} \tag{2.94}$$

and the projection onto the odd subspace is

$$Q\hat{\Omega} = \begin{cases} 0 & \text{if } g \le h,\\ \hat{\Omega} & \text{otherwise.} \end{cases} \tag{2.95}$$

Again, irrespective of N being even or odd, the energy of the ground state of the Hamiltonian H_Q can be expressed as

$$E_0^{(Q)} = -\frac{1}{2}\sum_{p\in Q_N} \omega_p\,. \tag{2.96}$$

For the rest of this section, we will restrict our attention to the case where $g > 0$ and $h > 0$. Under this assumption, the identities in (2.88), (2.90), (2.93), and (2.95) for the projections of the ground states of H_P and H_Q reduce to

$$P\tilde{\Omega} = \tilde{\Omega}\,, \tag{2.97}$$

$$Q\hat{\Omega} = \begin{cases} 0 & \text{if } g \leq h, \\ \hat{\Omega} & \text{otherwise,} \end{cases} \tag{2.98}$$

and, therefore, become independent of N.

For any N, the energy of the ground state of H_P is smaller than the energy of the ground state of H_Q. Additionally, the projection of the ground state of H_P onto the even subspace is non-zero. In particular, we have observed that $P\tilde{\Omega} = \tilde{\Omega}$. Therefore, according to our considerations at the end of Section 2.2, the ground state of the transverse Ising chain, Ω, equals to $\tilde{\Omega}$ and the energy of the ground state, E_0, is given by the ground state energy $E_0^{(P)}$ of H_P. The ground state is non-degenerate. [1]

For any finite N, the ground state energy density of H_P,

$$\frac{E_0^{(P)}}{N} = -\frac{1}{N}\sum_{p\in P_N}\sqrt{g^2+h^2-2gh\cos p}\,, \tag{2.99}$$

is the middle Riemann sum, and the ground state energy density of H_Q,

$$\frac{E_0^{(Q)}}{N} = -\frac{1}{N}\sum_{p\in Q_N}\sqrt{g^2+h^2-2gh\cos p}\,, \tag{2.100}$$

is the left Riemann sum of the integral of the function

$$[-\pi,\pi] \longrightarrow \mathbb{R},\; p \mapsto -\frac{1}{2\pi}\sqrt{g^2+h^2-2gh\cos p}\,. \tag{2.101}$$

Therefore, the thermodynamic limit, $N \to \infty$, of the ground state energy densities exists and they converge to the same value

$$\varepsilon_0 \coloneqq -\frac{1}{2\pi}\int_{-\pi}^{\pi}\sqrt{g^2+h^2-2gh\cos p}\,\mathrm{d}p\,. \tag{2.102}$$

But then, the identities in (2.97) and (2.98) together with the consideration at the end of the Section 2.2 imply that, in the thermodynamic limit, whereas for $h \geq g$ the ground state of the transverse field Ising chain is still non-degenerate and given by

[1] We could not prove that the ground state energy of H_P is always smaller than the ground state energy of H_Q for any N. However, numerical results suggest that this claim holds. Additionally, in [Calabrese et al., 2012a], it is stated that the ground state of the transverse Ising chain is given by the ground state of H_P, though, the authors do not provide a proof of this claim.

$\tilde{\Omega}$, for $0 < h < g$, the ground state is represented by a linear combination of $\tilde{\Omega}$ and $\hat{\Omega}$ and is, thus, degenerate. While P commutes with the Hamiltonian and leaves the ground state invariant for any finite N, this is no longer true in the thermodynamic limit for $0 < h < g$. Then, the ground state is given by a superposition of $\tilde{\Omega}$ and $\hat{\Omega}$ and, thus, is no longer invariant under P. The symmetry is spontaneously broken. This already indicates that at $h = g$ there is a quantum critical point.

A quantum critical point is a point of non-analycity of the ground state energy density in the thermodynamic limit, which is for the transverse field Ising chain given by the expression (2.102). For fixed $g > 0$ we consider the ground state energy density as a function of $h > 0$. If

$$E(k) = \int_0^{\frac{\pi}{2}} \sqrt{1 - k^2 \sin^2(p)}\, \mathrm{d}p$$

denotes the complete elliptic integral of second kind, then the ground state energy density in the thermodynamic limit can be expressed as

$$\varepsilon_0(h) = -\frac{2}{\pi}(g+h)E\left(\sqrt{\frac{4gh}{(g+h)^2}}\right) . \tag{2.103}$$

This function has a point of non-analycity for $g = h$. Therefore, the trasverse Ising chain has a quantum critical point at $g = h$ and exhibits a quantum phase transition. For $h < g$, the system is ferromagnetic, whereas for $h > g$ it is paramagnetic. The order parameter is given by the expectation values of the operators X_j with respect to the ground state of the transverse Ising chain, which are independent of the site on the chain due to the periodic boundary condition. We will call the operator X_j itself the order parameter from now on. In the thermodynamic limit, it is non-zero in the ferromagnetic phase due to the spontaneous symmetry breaking.

3 Ground State Correlation Functions

Our objective in this chapter is to determine the correlation functions of the Pauli operators on the compound Hilbert space, $\mathcal{H}_N$, with respect to the ground state of the transverse Ising chain. These correlation functions are explicitly given by $\langle \Omega | X_j X_k \Omega \rangle$, $\langle \Omega | Y_j Y_k \Omega \rangle$, and $\langle \Omega | Z_j Z_k \Omega \rangle$ for any $j, k \in \{0, 1, \ldots, N-1\}$, where Ω is the ground state of the transverse Ising chain, which we have determined in Section 2.5. We will call them the ground state correlators for short. In calculating these ground state correlators, we will rely on a method which has been applied by Lieb, Schultz, and Mattis in [Lieb et al., 1961] to obtain the ground state correlation functions for the simple XY model. The result will be that the ground state correlators are given by determinants of Toeplitz matrices.

For determinants of a particular type of Toeplitz matrices, there are theorems which can be used to obtain the behaviour of the determinant for large sizes of the matrix analytically. We will use theorems proven in [Böttcher and Widom, 2006] by Albrecht Böttcher and Harold Widom, and which we summarized in the Appendix B, to obtain analytic expressions for the correlation function of the order parameter, X_j, in the thermodynamic limit, $N \to \infty$.

There are two reasons for us to consider the ground state correlators. The first reason is that we can understand the properties of the ground state in more detail. In particular, we will be able to determine the magnetization in the ferromagnetic phase, which is the order parameter of the quantum phase transition. The second reason is that in the calculations of these correlators, we will introduce methods which will be used later to determine correlations after sudden quenches. We introduce these methods here because the calculations are simpler, which allows us to clearly lay out the logic.

For the remainder of this chapter, we take g and h to be positive.

3.1 Finite Size Systems

We begin our considerations by determining the ground state correlators for a finite and fixed value of N. We found in Section 2.5 that Ω can be chosen to be $\tilde{\Omega}$, where $\tilde{\Omega}$ represents the ground state of H_P and the vacuum state of the Bogoliubov operators c_p for $p \in P_N$. Therefore, we use $\Omega = \tilde{\Omega}$.

Since Ω represents the vacuum state of the fermionic Bogoliubov operators c_p for $p \in P_N$, we can use the following implication of Wick's theorem: Let $\Psi_1, \Psi_2, \ldots, \Psi_{2n}$ be mutually anticommuting operators and let $\mathfrak{S}_{2n}$ denote the symmetric group of degree $2n$. Then, we have that

$$\langle \Omega | \Psi_1 \Psi_2 \cdots \Psi_{2n} \Omega \rangle = \frac{1}{2^n n!} \sum_{\sigma \in \mathfrak{S}_{2n}} \operatorname{sign} \sigma \prod_{j=1}^{n} \left\langle \Omega \middle| \Psi_{\sigma(2j-1)} \Psi_{\sigma(2j)} \Omega \right\rangle . \tag{3.1}$$

This expression is the Pfaffian, $\operatorname{pf} C$, of the antisymmetric contraction matrix, C, which is given by

$$C_{lm} := \begin{cases} \langle \Omega | \Psi_l \Psi_m \Omega \rangle & \text{if } l \neq m, \\ 0 & \text{otherwise,} \end{cases} \tag{3.2}$$

for all $l, m \in \{1, 2, \ldots, 2n\}$. Therefore, the idea is to express $X_j X_k$, $Y_j Y_k$, and $Z_j Z_k$ as a product of mutually anticommuting operators and use Wick's theorem to express the ground state correlators as functions of two-point correlation functions.

We only need to consider $X_j X_k$, $Y_j Y_k$, and $Z_j Z_k$ for $j, k \in \{0, 1, \ldots, N-1\}$ with $j < k$. For $j = k$, the products reduce to squares of the Pauli operators, which are the identity operator. For $j > k$, we can commute the Pauli operators and interchange the labels j and k, which reduces this case to the first one.

Let $j, k \in \{0, 1, \ldots, N-1\}$ with $j < k$. Using the expressions for the Pauli operators in terms of the Jordan-Wigner operators given in (2.19), (2.20), and (2.21), we obtain that

$$\begin{aligned} X_j X_k &= \left(a_j^\dagger + a_j \right) \exp\left(\mathrm{i}\pi \sum_{l=j}^{k-1} a_l^\dagger a_l \right) \left(a_k^\dagger + a_k \right) , \\ Y_j Y_k &= -\left(a_j^\dagger - a_j \right) \exp\left(\mathrm{i}\pi \sum_{l=j}^{k-1} a_l^\dagger a_l \right) \left(a_k^\dagger - a_k \right) , \\ Z_j Z_k &= \left(I - 2 a_j^\dagger a_j \right) \left(I - 2 a_k^\dagger a_k \right) . \end{aligned}$$

We can rewrite these expressions in terms of the operators A_l and B_l introduced in (2.22) and (2.23). To this end, we use (2.17) and (2.27) in conjunction with the anticommutation relations for A_l and B_l, which are given in (2.24), (2.25), and (2.26), to obtain that

$$X_j X_k = (-1)^{r(r-1)/2} B_j B_{j+1} \cdots B_{k-1} A_{j+1} A_{j+2} \cdots A_k , \tag{3.3}$$

$$Y_j Y_k = (-1)^{r(r-1)/2} B_{j+1} B_{j+2} \cdots B_k A_j A_{j+1} \cdots A_{k-1} , \tag{3.4}$$

$$Z_j Z_k = -B_j B_k A_j A_k . \tag{3.5}$$

We find that these expressions for $X_j X_k$, $Y_j Y_k$, and $Z_j Z_k$ involve only products of mutually anticommuting operators. Therefore, we can use the Equation (3.1) to determine the ground state correlators.

For any $j, k \in \{0, 1, \ldots, N-1\}$, let

$$G_{jk} \coloneqq \langle \Omega | B_j A_k \Omega \rangle \ , \tag{3.6}$$
$$Q_{jk} \coloneqq \langle \Omega | A_j A_k \Omega \rangle \ , \tag{3.7}$$
$$S_{jk} \coloneqq \langle \Omega | B_j B_k \Omega \rangle \ . \tag{3.8}$$

Since we are considering periodic boundary conditions, the system is translationally invariant. Therefore, the expressions G_{jk}, Q_{jk}, and S_{jk} can only depend on the relative distance on the chain. Consequently, there are expressions g_m, q_m, and s_m for $m \in \mathbb{Z}$ such that

$$G_{jk} = g_{k-j} \ , \tag{3.9}$$
$$Q_{jk} = q_{k-j} \ , \tag{3.10}$$
$$S_{jk} = s_{k-j} \ . \tag{3.11}$$

Thus, combining (3.3) and (3.4) with (3.1), we obtain with the above definitions that

$$\langle \Omega | X_0 X_r \Omega \rangle = (-1)^{r(r-1)/2} \operatorname{pf} \begin{bmatrix} 0 & s_1 & s_2 & \cdots & s_{r-1} & g_1 & g_2 & \cdots & g_r \\ & 0 & s_1 & \cdots & s_{r-2} & g_0 & g_1 & \cdots & g_{r-1} \\ & & \ddots & \ddots & \vdots & \vdots & \vdots & & \vdots \\ & & & 0 & s_1 & g_{-r+3} & g_{-r+4} & \cdots & g_2 \\ & & & & 0 & g_{-r+2} & g_{-r+3} & \cdots & g_1 \\ & & & & & 0 & q_1 & \cdots & q_{r-1} \\ & & & & & & \ddots & \ddots & \vdots \\ & & & & & & & 0 & q_1 \\ & & & & & & & & 0 \end{bmatrix} , \tag{3.12}$$

$$\langle \Omega | Y_0 Y_r \Omega \rangle = (-1)^{r(r-1)/2} \operatorname{pf} \begin{bmatrix} 0 & s_1 & s_2 & \cdots & s_{r-1} & g_{-1} & g_0 & \cdots & g_{r-2} \\ & 0 & s_1 & \cdots & s_{r-2} & g_{-2} & g_{-1} & \cdots & g_{r-3} \\ & & \ddots & \ddots & \vdots & \vdots & \vdots & & \vdots \\ & & & 0 & s_1 & g_{-r+1} & g_{-r+2} & \cdots & g_0 \\ & & & & 0 & g_{-r} & g_{-r+1} & \cdots & g_{-1} \\ & & & & & 0 & q_1 & \cdots & q_{r-1} \\ & & & & & & \ddots & \ddots & \vdots \\ & & & & & & & 0 & q_1 \\ & & & & & & & & 0 \end{bmatrix} , \tag{3.13}$$

for any $r \in \{1, \ldots, N-1\}$, where we only have written the upper triangular parts of the antisymmetric matrices since the lower triangular parts are the negatives of the transposes of the corresponding upper triangular parts[1]. The last correlator can be evaluated directly from (3.5), which gives

$$\langle \Omega | Z_0 Z_r \Omega \rangle = g_0^2 - g_r g_{-r} - s_r q_r \,. \tag{3.14}$$

In order to determine g_m, q_m, and s_m for $m \in \mathbb{Z}$, we need to calculate G_{jk}, Q_{jk}, and S_{jk} for any $j, k \in \{0, 1, \ldots, N-1\}$. To do so, we need to express the Jordan-Wigner operators, which are given by (2.7), in terms of the fermionic Bogoliubov operators c_p and $c_p^\dagger$ where $p \in P_N$.

Using the inversions of the Fourier and Bogoliubov transformations, we obtain

$$a_j = \frac{1}{\sqrt{N}} \sum_{p \in P_N} b_p e^{\mathrm{i}pj} = \frac{1}{\sqrt{N}} \sum_{p \in P_N} \left(u_p^* c_p + v_p^* c_{-p}^\dagger \right) e^{\mathrm{i}pj} \,.$$

If N is even, we have that

$$P_N = \frac{2\pi}{N} \left\{ -\frac{N-1}{2}, -\frac{N-3}{2}, \ldots, \frac{N-1}{2} \right\} \,.$$

Thus, we obtain that

$$\sum_{p \in P_N} v_p^* e^{\mathrm{i}pj} c_{-p}^\dagger = \sum_{p \in P_N} v_{-p}^* e^{-\mathrm{i}pj} c_p^\dagger \,.$$

If N is odd, we have that

$$P_N = \frac{2\pi}{N} \left\{ -\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1 \right\} \,.$$

In this case, we need to consider $v_p^* e^{\mathrm{i}pj} c_{-p}^\dagger$ for $p = -\pi$ separately. We can use the 2π-periodicity of the invoved terms to obtain that

$$v_{-\pi}^* e^{\mathrm{i}\pi j} c_\pi^\dagger = v_{-\pi+2\pi}^* e^{\mathrm{i}(\pi - 2\pi)j} c_{\pi-2\pi}^\dagger = v_\pi^* e^{-\mathrm{i}\pi j} c_{-\pi}^\dagger \,.$$

Therefore, we, again, obtain that

$$\sum_{p \in P_N} v_p^* e^{\mathrm{i}pj} c_{-p}^\dagger = \sum_{p \in P_N} v_{-p}^* e^{-\mathrm{i}pj} c_p^\dagger \,.$$

In summary, we can rewrite a_j in terms of the fermionic Bogoliubov operators as

$$a_j = \sum_{p \in P_N} \left(u_{pj}^* c_p + v_{pj} c_p^\dagger \right) \,, \tag{3.15}$$

[1] The correlator $\langle \Omega | X_0 X_r \Omega \rangle$ has been also calculated in [Barouch and McCoy, 1971a]. However, there, the factor $(-1)^{r(r-1)/2}$ is missing in the result.

with

$$u_{pj} := \frac{1}{\sqrt{N}} u_p e^{-\mathrm{i}pj} \,, \tag{3.16}$$

$$v_{pj} := \frac{1}{\sqrt{N}} v_{-p}^* e^{-\mathrm{i}pj} \,. \tag{3.17}$$

We use this expression for a_j to write the operators $A_j = a_j^\dagger + a_j$ and $B_j = a_j^\dagger - a_j$ in terms of the fermionic Bogoliubov operators as

$$A_j = \sum_{p \in P_N} \Big((u_{pj} + v_{pj}) c_p^\dagger + (u_{pj}^* + v_{pj}^*) c_p \Big) \,, \tag{3.18}$$

$$B_j = \sum_{p \in P_N} \Big((u_{pj} - v_{pj}) c_p^\dagger - (u_{pj}^* - v_{pj}^*) c_p \Big) \,. \tag{3.19}$$

Since $c_p \Omega = 0$ for all $p \in P_N$, we obtain that

$$\begin{aligned} G_{jk} &= \sum_{p \in P_N} (v_{pj}^* - u_{pj}^*)(u_{pk} + v_{pk}) \,, \\ Q_{jk} &= \sum_{p \in P_N} (v_{pj}^* + u_{pj}^*)(u_{pk} + v_{pk}) \,, \\ S_{jk} &= \sum_{p \in P_N} (v_{pj}^* - u_{pj}^*)(u_{pk} - v_{pk}) \,. \end{aligned}$$

for all $j, k \in \{0, 1, \ldots, N-1\}$. By using the expressions for u_{pj} and v_{pj} given in (3.16) and (3.17), and simplifying the resulting expressions, we obtain that

$$G_{jk} = -\frac{1}{N} \sum_{p \in P_N} \Big(|u_p|^2 - |v_p|^2 - 2\mathrm{i}\, \mathrm{Im}(u_p v_{-p}) \Big) \, e^{-\mathrm{i}p(k-j)} \,,$$

and that

$$Q_{jk} = \delta_{jk} = -S_{jk} \,.$$

Therefore, we have that

$$g_m := -\frac{1}{N} \sum_{p \in P_N} \Big(|u_p|^2 - |v_p|^2 - 2\mathrm{i}\, \mathrm{Im}(u_p v_{-p}) \Big) \, e^{-\mathrm{i}pm} \,, \tag{3.20}$$

and

$$q_m := \delta_{m = 0 \bmod N} \,, \tag{3.21}$$

$$s_m := -\delta_{m = 0 \bmod N} \,, \tag{3.22}$$

for all $m \in \mathbb{Z}$.

As an immediate consequence, the blocks in the Pfaffian expressions in (3.12) and (3.13) involving q_m and s_m vanish. This allows us to simplify these correlators since the Pfaffian has the following property: Let M denote an arbitrary n by n matrix for some positive integer n. Then, we have that

$$\operatorname{pf}\begin{bmatrix} 0 & M \\ -M^{\mathrm{T}} & 0 \end{bmatrix} = (-1)^{n(n-1)/2} \det M \,. \tag{3.23}$$

With that, we arrive at the final result for the correlation functions,

$$\langle \Omega | X_0 X_r \Omega \rangle = \det \begin{bmatrix} g_1 & g_2 & \cdots & g_r \\ g_0 & g_1 & \cdots & g_{r-1} \\ \vdots & \vdots & & \vdots \\ g_{-r+3} & g_{-r+4} & \cdots & g_2 \\ g_{-r+2} & g_{-r+3} & \cdots & g_1 \end{bmatrix} , \tag{3.24}$$

and

$$\langle \Omega | Y_0 Y_r \Omega \rangle = \det \begin{bmatrix} g_{-1} & g_0 & \cdots & g_{r-2} \\ g_{-2} & g_{-1} & \cdots & g_{r-3} \\ \vdots & \vdots & & \vdots \\ g_{-r+1} & g_{-r+2} & \cdots & g_0 \\ g_{-r} & g_{-r+1} & \cdots & g_{-1} \end{bmatrix} , \tag{3.25}$$

and for the last correlator, we obtain that

$$\langle \Omega | Z_0 Z_r \Omega \rangle = g_0^2 - g_r g_{-r} + \delta_{r=0 \bmod N} \tag{3.26}$$

for any $r \in \{1, 2, \ldots, N-1\}$.

This completes the calculation of the ground state correlation functions of the Pauli operators. We observe that the ground state correlators of the X_j and Y_j operators are given by determinants of Toeplitz matrices. This will allow us to consider the asymptotic behaviour for large relative separations, r, in the thermodynamic limit and allows also an efficient numerical evaluation for finite chains.

3.2 The Thermodynamic Limit

We will now consider the thermodynamic limit, $N \to \infty$. We will restrict ourselves only to the correlation function of the order parameter X_j since the same reasoning will apply for the other correlators. Let C_r denote the correlation function of the order parameter with respect to the ground state of the transverse Ising chain in the thermodynamic limit.

To analyze the thermodynamic limit, we make the dependencies on the chain size, N, explicit. The even and odd parts of the Hamiltonian, H_P and H_Q, depend on N and their respective ground states depend on N as well. We will denote their representatives by $\tilde{\Omega}_N$ and $\hat{\Omega}_N$, respectively.

As we will see, we need to calculate $\left\langle \tilde{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle$ and $\left\langle \hat{\Omega}_N \middle| X_0 X_r \hat{\Omega}_N \right\rangle$ for any $r \in \{1, 2, \ldots, N-1\}$. The first one of them, $\left\langle \tilde{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle$, has been calculated in the preceding section. However, in order to keep the notations unified, we rewrite the result to make the dependence on N explicit. To this end, for any $m \in \mathbb{Z}$, let

$$\tilde{g}_{N,m} := -\frac{1}{N} \sum_{p \in P_N} \left(|u_p|^2 - |v_p|^2 - 2\mathrm{i}\,\mathrm{Im}(u_p v_{-p}) \right) e^{-\mathrm{i}pm} . \tag{3.27}$$

Then, we have that

$$\left\langle \tilde{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle = \det \begin{bmatrix} \tilde{g}_{N,1} & \tilde{g}_{N,2} & \cdots & \tilde{g}_{N,r} \\ \tilde{g}_{N,0} & \tilde{g}_{N,1} & \cdots & \tilde{g}_{N,r-1} \\ \vdots & \vdots & & \vdots \\ \tilde{g}_{N,-r+3} & \tilde{g}_{N,-r+4} & \cdots & \tilde{g}_{N,2} \\ \tilde{g}_{N,-r+2} & \tilde{g}_{N,-r+3} & \cdots & \tilde{g}_{N,1} \end{bmatrix} . \tag{3.28}$$

The correlation function $\left\langle \hat{\Omega}_N \middle| X_0 X_r \hat{\Omega}_N \right\rangle$ can be obtained using Wick's theorem as well since $\hat{\Omega}_N$ represents the vacuum state of the fermionic Bogoliubov operators c_p for $p \in Q_N$. Introducing

$$\hat{g}_{N,m} := -\frac{1}{N} \sum_{p \in Q_N} \left(|u_p|^2 - |v_p|^2 - 2\mathrm{i}\,\mathrm{Im}(u_p v_{-p}) \right) e^{-\mathrm{i}pm} . \tag{3.29}$$

for any $m \in \mathbb{Z}$, we obtain that

$$\left\langle \hat{\Omega}_N \middle| X_0 X_r \hat{\Omega}_N \right\rangle = \det \begin{bmatrix} \hat{g}_{N,1} & \hat{g}_{N,2} & \cdots & \hat{g}_{N,r} \\ \hat{g}_{N,0} & \hat{g}_{N,1} & \cdots & \hat{g}_{N,r-1} \\ \vdots & \vdots & & \vdots \\ \hat{g}_{N,-r+3} & \hat{g}_{N,-r+4} & \cdots & \hat{g}_{N,2} \\ \hat{g}_{N,-r+2} & \hat{g}_{N,-r+3} & \cdots & \hat{g}_{N,1} \end{bmatrix} . \tag{3.30}$$

The deriviation is in complete analogy to Section 3.1. In fact, the only difference is the choice of momenta in the sum (3.29).

In the paramagnetic phase and at the quantum critical point, where $h \geq g$, the ground state of the transverse Ising chain remains non-degenerate even in the thermodynamic limit, as we observed in the Section 2.5. Therefore, we obtain that

$$C_r = \lim_{N \to \infty} \left\langle \tilde{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle$$

for $h \geq g$.

In the ferromagnetic phase, where $h < g$, the ground state of the transverse Ising chain is degenerate. It is represented by any superposition of the ground states of the even and the odd parts of the Hamiltonian, as we saw in the Section 2.5. In order to obtain the correlator of the order parameter with respect to the ground state in the thermodynamic limit within the ferromagnetic phase, we need to determine the correlation function with respect to the state represented by $\alpha\tilde{\Omega}_N + \beta\hat{\Omega}_N$, where α and β are complex numbers for which $|\alpha|^2 + |\beta|^2 = 1$ and, then, take the limit $N \to \infty$ of the resulting expression. We obtain that

$$\begin{aligned}\left\langle \alpha\tilde{\Omega}_N + \beta\hat{\Omega}_N \middle| X_0 X_r \left(\alpha\tilde{\Omega}_N + \beta\hat{\Omega}_N\right)\right\rangle \\ = |\alpha|^2 \left\langle \tilde{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle + \alpha^*\beta \left\langle \tilde{\Omega}_N \middle| X_0 X_r \hat{\Omega}_N \right\rangle \\ + \beta^*\alpha \left\langle \hat{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle + |\beta|^2 \left\langle \hat{\Omega}_N \middle| X_0 X_r \hat{\Omega}_N \right\rangle . \end{aligned} \quad (3.31)$$

Since $\tilde{\Omega}_N \in P(\mathcal{H}_N)$ and $\hat{\Omega}_N \in Q(\mathcal{H}_N)$, we have that $X_0 X_r \tilde{\Omega}_N \in P(\mathcal{H}_N)$ and $X_0 X_r \hat{\Omega}_N \in Q(\mathcal{H}_N)$. This can be seen by using the characterizations of the even and the odd subspaces in terms of the eigenvectors of the Pauli operators Z_j, χ_s with $s \in \{0,1\}^N$ which are given in (2.40), as we described in Section 2.2. There, we saw that elements in $P(\mathcal{H}_N)$ and elements in $Q(\mathcal{H}_N)$ are linear combinations of χ_s which represent an even and, respectively, odd number of spin-down states. The claim follows from the observation that the operators $X_0 X_r$ flip spins at two sites. Since $P(\mathcal{H}_N)$ and $Q(\mathcal{H}_N)$ are mutually orthogonal, we obtain that $\left\langle \tilde{\Omega}_N \middle| X_0 X_r \hat{\Omega}_N \right\rangle = 0 = \left\langle \hat{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle$. What remains is the expression

$$\begin{aligned}\left\langle \alpha\tilde{\Omega}_N + \beta\hat{\Omega}_N \middle| X_0 X_r \left(\alpha\tilde{\Omega}_N + \beta\hat{\Omega}_N\right)\right\rangle \\ = |\alpha|^2 \left\langle \tilde{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle + |\beta|^2 \left\langle \hat{\Omega}_N \middle| X_0 X_r \hat{\Omega}_N \right\rangle . \end{aligned} \quad (3.32)$$

We need to determine the limits of $\left\langle \tilde{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle$ and $\left\langle \hat{\Omega}_N \middle| X_0 X_r \hat{\Omega}_N \right\rangle$ as $N \to \infty$. For this purpose, note that, for any $m \in \mathbb{Z}$, $\tilde{g}_{N,m}$ and $\hat{g}_{N,m}$ are Riemann sums of the integral of the function

$$[-\pi, \pi] \longrightarrow \mathbb{C},\ p \mapsto -\frac{1}{2\pi}\left(|u_p|^2 - |v_p|^2 - 2\mathrm{i}\,\mathrm{Im}(u_p v_{-p})\right) e^{-\mathrm{i}pm} .$$

Therefore, we have that

$$\lim_{N\to\infty} \tilde{g}_{N,m} = \lim_{N\to\infty} \hat{g}_{N,m} .$$

Since the determinant is a continuous function of the entries of the matrix, this implies that

$$\lim_{N\to\infty} \left\langle \tilde{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle = \lim_{N\to\infty} \left\langle \hat{\Omega}_N \middle| X_0 X_r \hat{\Omega}_N \right\rangle .$$

Since $|\alpha|^2 + |\beta|^2 = 1$, this, in turn, gives that

$$C_r = \lim_{N\to\infty} \left\langle \tilde{\Omega}_N \middle| X_0 X_r \tilde{\Omega}_N \right\rangle .$$

After this formal treatment of the different phases, we are now in the position to derive the thermodynamic limit of the correlation function. For any $m \in \mathbb{Z}$, let $g_m \coloneqq \lim_{N\to\infty} \tilde{g}_{N,m}$. Since $\tilde{g}_{N,m}$ converges to g_m for all $m \in \mathbb{Z}$, any subsequence of $\tilde{g}_{N,m}$ converges to g_m as well. Therefore, we consider $\tilde{g}_{N,m}$ only for even N. In that case, by using the definitions of u_p and v_p given in (2.74) and (2.75), we obtain that

$$\tilde{g}_{N,m} = \frac{1}{N} \sum_{p\in P_N} \frac{e^{\mathrm{i}p} - \lambda}{\sqrt{1+\lambda^2 - 2\lambda\cos p}} e^{-\mathrm{i}pm} ,$$

where we introduced $\lambda \coloneqq h/g$. Thus, we have for the limit that

$$g_m = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{\mathrm{i}p} - \lambda}{\sqrt{1+\lambda^2 - 2\lambda\cos p}} e^{-\mathrm{i}pm} \, \mathrm{d}p , \tag{3.33}$$

for all $m \in \mathbb{Z}$.

We can now express C_r as a determinant of a r by r Toeplitz matrix whose entries are given by g_m. However, to rewrite the Toeplitz matrix in a conventional form and in order to match the notation used in the Appendix B, we define $f_m \coloneqq g_{1-m}$ for all $m \in \mathbb{Z}$. For all $m \in \mathbb{Z}$,

$$f_m = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1 - \lambda e^{\mathrm{i}p}}{\sqrt{1+\lambda^2 - 2\lambda\cos p}} e^{-\mathrm{i}pm} \, \mathrm{d}p . \tag{3.34}$$

We see that the f_m are given by a Fourier transform. To make this point more explicit, we define on the complex unit circle, $S^1 = \{z \in \mathbb{C} \,|\, |z| = 1\}$, the function

$$f : S^1 \longrightarrow \mathbb{C},\; z \mapsto f(z) \coloneqq \frac{1 - \lambda z}{\sqrt{1 + \lambda^2 - \lambda\left(z + \frac{1}{z}\right)}} .$$

Then, we obtain that

$$f_m = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(e^{\mathrm{i}p}) e^{-\mathrm{i}pm} \, \mathrm{d}p ,$$

for all $m \in \mathbb{Z}$. For any positive integer r, we can write C_r as the determinant of the r by r Toeplitz matrix generated by f, namely

$$C_r = \det \begin{bmatrix} f_0 & f_{-1} & \cdots & f_{-r+1} \\ f_1 & f_0 & \cdots & f_{-r+2} \\ \vdots & \vdots & & \vdots \\ f_{r-2} & f_{r-3} & \cdots & f_{-1} \\ f_{r-1} & f_{r-2} & \cdots & f_0 \end{bmatrix} . \tag{3.35}$$

3.3 Asymptotics of the Order Parameter Correlator

To determine the asymptotic behaviour of the order parameter ground state correlator in the thermodynamic limit, C_r, for large values of the relative separation, r, we will use the theorems summarized in the Appendix B. First, we need to analyse the function f. Namely, we need to show that the function f is a continuous function which is nowhere zero and that f is in C^β for some $\beta > 1/2$ and $\beta \notin \mathbb{N}$, which means that f has $\lfloor\beta\rfloor$ continuous derivatives and that the $\lfloor\beta\rfloor$th derivative is Hölder continuous with the exponent $\beta - \lfloor\beta\rfloor$. Whether we need Theorem B.1 or Theorem B.2 will depend on the winding number of f about zero.

For $\lambda \neq 1$, the function f is continuous and nowhere zero on S^1. This can be seen as follows. Let $\lambda \neq 1$. The functions given by $1 - \lambda z$ and $\sqrt{1 + \lambda^2 - \lambda(z + 1/z)}$ are continuous on the unit circle, S^1. For any $z \in S^1$, there is a $p \in [-\pi, \pi[$ such that $z = e^{\mathrm{i}p}$. Therefore, we obtain that

$$\sqrt{1 + \lambda^2 - \lambda\left(z + \frac{1}{z}\right)} = \sqrt{1 + \lambda^2 - 2\lambda\cos p}\,.$$

Furthermore, we have that $1 + \lambda^2 - 2\lambda\cos p > 0$ since $(1-\lambda)^2 > 0$ is equivalent to $1 + \lambda^2 > 2\lambda$ and since $-1 \leq \cos p \leq 1$, we obtain that $1 + \lambda^2 > 2\lambda\cos p$. Thus, $\sqrt{1 + \lambda^2 - \lambda(z + 1/z)} > 0$ for all $z \in S^1$. Therefore, we obtain that f is continuous. Since we also have $|\lambda z| = \lambda \neq 1$ for all $z \in S^1$, f is also nowhere zero on S^1.

For $\lambda = 1$, the function f takes the form

$$f(z) = \frac{1 - z}{\sqrt{2 - \left(z + \frac{1}{z}\right)}}$$

for all $z \in S^1$. The functions is non-zero and continuous if $z \neq 1$. However, it is not continuous at $z = 1$. This can be seen as follows. We can write $f(e^{\mathrm{i}p})$ as

$$f(e^{\mathrm{i}p}) = \frac{1}{\sqrt{2}}\left(\frac{1 - \cos p}{\sqrt{1 - \cos p}} - \mathrm{i}\frac{\sin p}{\sqrt{1 - \cos p}}\right),$$

for $p \in [-\pi, \pi[$ and $p \neq 0$. For $0 < p < \pi$, $\sin p$ is non-negative and we obtain that

$$\operatorname{Im} f(e^{\mathrm{i}p}) = -\frac{1}{\sqrt{2}}\frac{\sin p}{\sqrt{1 - \cos p}} = -\frac{1}{\sqrt{2}}\sqrt{\frac{\sin^2 p}{1 - \cos p}} = -\sqrt{\frac{1 + \cos p}{2}}\,.$$

For $-\pi \leq p < 0$, $\sin p$ is non-positive and we obtain that

$$\operatorname{Im} f(e^{\mathrm{i}p}) = -\frac{1}{\sqrt{2}}\frac{\sin p}{\sqrt{1 - \cos p}} = \frac{1}{\sqrt{2}}\sqrt{\frac{\sin^2 p}{1 - \cos p}} = \sqrt{\frac{1 + \cos p}{2}}\,.$$

Therefore, we have that

$$\lim_{\substack{p\to 0\\ 0<p<\pi}} \operatorname{Im} f(e^{\mathrm{i}p}) = -\lim_{\substack{p\to 0\\ 0<p<\pi}} \sqrt{\frac{1+\cos p}{2}} = -1\,,$$

$$\lim_{\substack{p\to 0\\ -\pi\le p<0}} \operatorname{Im} f(e^{\mathrm{i}p}) = \lim_{\substack{p\to 0\\ -\pi\le p<0}} \sqrt{\frac{1+\cos p}{2}} = 1\,.$$

Thus, f is not continuous at $z = 1$. However, in order to be able to use the Theorems B.1 and B.2, which are given in the Appendix B, we need f to be continuous and nowhere zero. Therefore, we restrict ourselves to $\lambda \neq 1$.

As already stated above, whether we can use Theorem B.1 or Theorem B.2 depends on the winding number of f about the origin. Therefore, before we check whether there is a $\beta > 1/2$ with $\beta \notin \mathbb{N}$ such that f is in C^β, let us determine this winding number. Let γ denote the winding number of f about the origin. We have that

$$\gamma = \frac{1}{2\pi\mathrm{i}} \int_{f(S^1)} \frac{\mathrm{d}z}{z}$$

To determine the winding number, we parametrize the curve $f(S^1)$ by

$$\varphi : [-\pi,\pi] \longrightarrow f(S^1),\; p \mapsto \varphi(p) := f(e^{\mathrm{i}p})$$

Then, we obtain

$$\gamma = \frac{1}{2\pi\mathrm{i}} \int_{-\pi}^{\pi} \frac{\varphi'(p)}{\varphi(p)}\,\mathrm{d}p = \frac{1}{2\pi\mathrm{i}} \int_{-\pi}^{\pi} \left(-\frac{\mathrm{i}\lambda e^{\mathrm{i}p}}{1-\lambda e^{\mathrm{i}p}} - \frac{\lambda \sin p}{1+\lambda^2 - 2\lambda\cos p} \right) \mathrm{d}p\,.$$

The function

$$[-\pi,\pi] \longrightarrow \mathbb{R},\; p \mapsto \frac{\lambda \sin p}{1+\lambda^2-2\lambda\cos p}$$

is an odd function. Therefore, its integral over the intervall $[-\pi,\pi]$ vanishes, which reduces γ to

$$\gamma = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\lambda e^{\mathrm{i}p}}{\lambda e^{\mathrm{i}p}-1}\,\mathrm{d}p\,.$$

We rewrite this expression as a countour integral, which gives that

$$\gamma = \frac{1}{2\pi\mathrm{i}} \int_{S^1} \frac{\lambda}{\lambda z - 1}\,\mathrm{d}z\,. \tag{3.36}$$

From this point on, we need to differentiate between the cases $\lambda < 1$ and $\lambda > 1$.

3.3.1 Asymptotics in the Ferromagnetic Phase

Assume that $\lambda < 1$, that is, consider the ferromagnetic phase. For all $z \in S^1$, we have that $|\lambda z| = \lambda < 1$. Therefore, we can use the geometric series to expand the integrand in (3.36). We obtain that

$$\gamma = -\frac{\lambda}{2\pi \mathrm{i}} \int_{S^1} \frac{1}{1-\lambda z} \, \mathrm{d}z = -\frac{\lambda}{2\pi \mathrm{i}} \sum_{n=0}^{\infty} \lambda^n \int_{S^1} z^n \, \mathrm{d}z = 0$$

since, for any non-negative integer n, the complex function $z \mapsto z^n$ is holomorphic and, thus, Cauchy's integral theorem gives that $\int_{S^1} z^n \, \mathrm{d}z = 0$. Therefore, we can apply Theorem B.1, given that f is in C^β for a $\beta > 1/2$ and $\beta \notin \mathbb{N}$.

The function φ is smooth, that is, it has derivatives of all orders. This can be seen using the quotient rule. A continuously differentiable function over a compact intervall is Lipschitz continuous, which, in turn, implies that the function is Hölder continuous for any exponent in $]0,1[$. Since φ is smooth, φ itself and any of its derivatives are Hölder continuous for any exponent in $]0,1[$. This implies that for any $\beta > 1/2$ with $\beta \notin \mathbb{N}$, φ has $\lfloor \beta \rfloor$ continuous derivatives and the $\lfloor \beta \rfloor$th derivative satisfies a Hölder condition with the exponent $\beta - \lfloor \beta \rfloor$. This means that f is in C^β for any $\beta > 1/2$ with $\beta \notin \mathbb{N}$.

The above statements allow us to use Szegö's strong limit theorem, which is Theorem B.1 in the Appendix B. There, we can see that we need to calculate the Fourier coefficients of $\log f$ in order to determine the asymptotic behaviour of C_r.

We determine the Fourier coefficients of $\log f$. For any $p \in [-\pi, \pi[$, we have, for the principal logarithm, that

$$\log f(e^{\mathrm{i}p}) = \log(1 - \lambda e^{\mathrm{i}p}) - \frac{1}{2} \log(1 + \lambda^2 - 2\lambda \cos p) \,.$$

We can write

$$1 + \lambda^2 - 2\lambda \cos p = (1 - \lambda e^{\mathrm{i}p})(1 - \lambda e^{-\mathrm{i}p}) \,.$$

Since the principal arguments of $1 - \lambda e^{\mathrm{i}p}$ and $(1 - \lambda e^{\mathrm{i}p})^* = 1 - \lambda e^{-\mathrm{i}p}$ add to zero, we obtain that

$$\log((1 - \lambda e^{\mathrm{i}p})(1 - \lambda e^{-\mathrm{i}p})) = \log(1 - \lambda e^{\mathrm{i}p}) + \log(1 - \lambda e^{-\mathrm{i}p}) \,.$$

Therefore, we obtain that

$$\log f(e^{\mathrm{i}p}) = \frac{1}{2} \log(1 - \lambda e^{\mathrm{i}p}) - \frac{1}{2} \log(1 - \lambda e^{-\mathrm{i}p}) \,.$$

For any $w \in \mathbb{C}$ with $|w| < 1$, we have that

$$\log(1 - w) = -\sum_{n=1}^{\infty} \frac{1}{n} w^n \,.$$

Since $|\lambda z| = \lambda < 1$ for any $z \in S^1$, we obtain that

$$\log f(e^{\mathrm{i}p}) = -\frac{1}{2}\sum_{n=1}^{\infty}\frac{\lambda^n}{n}e^{inp} + \frac{1}{2}\sum_{n=1}^{\infty}\frac{\lambda^n}{n}e^{-inp}$$

By comparing this identity with the Fourier expansion

$$\log f(e^{\mathrm{i}p}) = \sum_{n=-\infty}^{\infty}(\log f)_n e^{inp}\,, \tag{3.37}$$

we obtain that

$$(\log f)_n = \begin{cases} -\frac{1}{2n}\lambda^n & \text{if } n \geq 1\,, \\ 0 & \text{if } n = 0\,, \\ -\frac{1}{2n}\lambda^{-n} & \text{if } n \leq -1\,. \end{cases} \tag{3.38}$$

Using these Fourier coefficients of $\log f$, we get that

$$\sum_{n=1}^{\infty} n(\log f)_{-n}(\log f)_n = -\frac{1}{4}\sum_{n=1}^{\infty}\frac{1}{n}\lambda^{2n} = \frac{1}{4}\log\left(1-\lambda^2\right)\,.$$

By applying Szegö's strong limit theorem (Theorem B.1), we obtain that

$$C_r = \left(1-\lambda^2\right)^{1/4}\left(1+\mathcal{O}\left(r^{1-2\beta}\right)\right)\,, \tag{3.39}$$

for all positive integers r and for any $\beta > 1/2$ with $\beta \notin \mathbb{N}$. This result allows us to determine the magnetization in the thermodynamic limit within the ferromagnetic phase. Namely, the cluster decomposition principle relates $\langle \Omega | X_0 \Omega \rangle$ to the correlator for large distances r by $C_r = \langle \Omega | X_0 \Omega \rangle^2$. Therefore, since the magnetization m_x is $\langle \Omega | X_0 \Omega \rangle /2$, we obtain that

$$m_x = \frac{1}{2}\left(1-\lambda^2\right)^{1/8}\,. \tag{3.40}$$

This result can be found in [Pfeuty, 1970] and it allows us to identify the critical exponent β' of the order parameter. Namely, we have that

$$\beta' = \lim_{\substack{\lambda\to 1 \\ \lambda<1}} \frac{\log\left(\frac{1}{2}\left(1-\lambda^2\right)^{1/8}\right)}{\log\left(1-\lambda\right)} = \frac{1}{8} \tag{3.41}$$

3.3.2 Asymptotics in the Paramagnetic Phase

Assume that $\lambda > 1$, that is, consider the paramagnetic phase. For all $z \in S^1$, we have that $|(\lambda z)^{-1}| = \lambda^{-1} < 1$. We rewrite the equation (3.36) in the form

$$\gamma = \frac{1}{2\pi\mathrm{i}}\int_{S^1}\frac{1/z}{1-\frac{1}{\lambda z}}\,\mathrm{d}z$$

and use the geometric series to obtain that

$$\frac{1}{1-\frac{1}{\lambda z}} = \sum_{n=0}^{\infty} \lambda^{-n} z^{-n} \,.$$

Therefore, we obtain that

$$\gamma = \sum_{n=0}^{\infty} \lambda^{-n} \frac{1}{2\pi \mathrm{i}} \int_{S^1} \frac{\mathrm{d}z}{z^{n+1}} = 1$$

since, for any non-negative integer n, Cauchy's integral formula gives

$$\frac{1}{2\pi \mathrm{i}} \int_{S^1} \frac{\mathrm{d}z}{z^{n+1}} = \delta_{n0} \,.$$

We cannot apply Theorem B.1 since $\gamma \neq 0$. We cannot apply Theorem B.2 either because γ is positive. However, we can use instead of f another function which generates the negative of the transposed Toeplitz matrix and has, thus, $-\gamma$ as its winding number about the origin. Namely, we introduce the new function

$$\hat{f} : S^1 \longrightarrow \mathbb{C},\ z \mapsto \hat{f}(z) \coloneqq -f(1/z) \,.$$

We also introduce

$$\hat{f}_m \coloneqq \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{f}(e^{\mathrm{i}p}) e^{-\mathrm{i}mp} \,\mathrm{d}p \,, \tag{3.42}$$

for all $m \in \mathbb{Z}$, with the property $\hat{f}_m = -f_{-m}$. For any positive integer r, let T_r and $\hat{T}_r$ denote the r by r Toeplitz matrices given by $(T_r)_{jk} = f_{j-k}$ and $(\hat{T}_r)_{jk} = \hat{f}_{j-k}$ for any $j, k \in \{0, 1, \ldots, r-1\}$. Since $\hat{f}_m = -f_{-m}$, we have that $\hat{T}_r = -T_r^{\mathrm{T}}$. Therefore, we obtain that

$$C_r = \det T_r = \det \left(-\hat{T}_r^{\mathrm{T}}\right) = (-1)^r \det \hat{T}_r \,.$$

In addition, we have that the winding number of $\hat{f}$ about zero is $-\gamma$ since $\hat{f}(e^{\mathrm{i}p}) = -f(e^{-\mathrm{i}p})$ and, thus, $\hat{f}$ circles the origin clockwise if f circles it counterclockwise and vice versa. Thus, the winding number of $\hat{f}$ about zero is -1.

Since $\hat{f}(z) = -f(1/z)$ for all $z \in S^1$, we have for the parametrization of $\hat{f}(S^1)$ given by

$$\hat{\varphi} : [-\pi, \pi] \longrightarrow \hat{f}(S^1),\ p \mapsto \hat{\varphi}(p) \coloneqq \hat{f}(e^{\mathrm{i}p})$$

that $\hat{\varphi}(p) = -\varphi(-p)$. Thus, it is smooth, which implies that, for any $\beta > 1/2$ with $\beta \notin \mathbb{N}$, the function has $\lfloor \beta \rfloor$ continuous derivatives and the $\lfloor \beta \rfloor$th derivative satisfies a Hölder condition with the exponent $\beta - \lfloor \beta \rfloor$. Therefore, we can apply the Theorem B.2.

To this end, define the function

$$a : S^1 \longrightarrow \mathbb{C},\ z \mapsto a(z) \coloneqq z\hat{f}(z) \,.$$

Explicitly, for all $z \in S^1$, we have that

$$a(z) = -\frac{z-\lambda}{\sqrt{1+\lambda^2-\lambda\left(z+\frac{1}{z}\right)}} = \frac{1-\lambda^{-1}z}{\sqrt{1+\lambda^{-2}-\lambda^{-1}\left(z+\frac{1}{z}\right)}}\,.$$

We observe that a has the same form as f with the difference being that we need to substitute λ in f by λ^{-1} to obtain a. Thus, since $\lambda^{-1} < 1$, we can obtain the Fourier coefficients of $\log a$ by substituting λ by λ^{-1} in the Fourier coefficients of $\log f$ obtained for $\lambda < 1$. Therefore, for any $p \in [-\pi, \pi[$, we have that

$$\log a(e^{\mathrm{i}p}) = \sum_{n=-\infty}^{\infty} (\log a)_n e^{\mathrm{i}np}\,, \tag{3.43}$$

with

$$(\log a)_n = \begin{cases} -\dfrac{1}{2n}\lambda^{-n} & \text{if } n \geq 1\,, \\ 0 & \text{if } n = 0\,, \\ -\dfrac{1}{2n}\lambda^{n} & \text{if } n \leq -1\,. \end{cases} \tag{3.44}$$

Further, we also have that

$$\sum_{n=1}^{\infty} n(\log a)_{-n}(\log a)_n = -\frac{1}{4}\sum_{n=1}^{\infty}\frac{1}{n}\lambda^{-2n} = \frac{1}{4}\log\left(1-\frac{1}{\lambda^2}\right)\,.$$

For the functions $a_\pm : S^1 \longrightarrow \mathbb{C}$ given by

$$a_\pm(z) \coloneqq \exp\left(\sum_{n=1}^{\infty}(\log a)_{\pm n} z^{\pm n}\right)$$

for all $z \in S^1$, we obtain that

$$a_+(e^{\mathrm{i}p}) = \exp\left(-\sum_{n=1}^{\infty}\frac{1}{2n}\left(\frac{e^{\mathrm{i}p}}{\lambda}\right)^n\right) = \exp\left(\frac{1}{2}\log\left(1-\frac{e^{\mathrm{i}p}}{\lambda}\right)\right) = \left(1-\frac{e^{\mathrm{i}p}}{\lambda}\right)^{1/2}\,,$$

and that

$$a_-(e^{\mathrm{i}p}) = \exp\left(\sum_{n=1}^{\infty}\frac{1}{2n}\left(\frac{e^{-\mathrm{i}p}}{\lambda}\right)^n\right) = \exp\left(-\frac{1}{2}\log\left(1-\frac{e^{-\mathrm{i}p}}{\lambda}\right)\right) = \left(1-\frac{e^{-\mathrm{i}p}}{\lambda}\right)^{-1/2}$$

for all $p \in [-\pi, \pi[$. In particular, we have that

$$\frac{a_-(e^{\mathrm{i}p})}{a_+(e^{\mathrm{i}p})} = \frac{\lambda}{\sqrt{1+\lambda^2-2\lambda\cos p}}\,.$$

By applying the theorem by Fisher, Hartwig, Silbermann et al. (Theorem B.2), we obtain that

$$C_r = \left(1-\frac{1}{\lambda^2}\right)^{1/4}\left(\frac{\lambda}{2\pi}\int_{-\pi}^{\pi}\frac{e^{-\mathrm{i}pr}}{\sqrt{1+\lambda^2-2\lambda\cos p}}\,\mathrm{d}p + \mathcal{O}\left(r^{-3\beta}\right)\right)\left(1+\mathcal{O}\left(r^{1-2\beta}\right)\right) \tag{3.45}$$

for all positive integers r and for any $\beta > 1/2$ with $\beta \notin \mathbb{N}$.

4 Correlations after a Sudden Quench

Quite often, the Hamiltonian of a system depends on some parameter, h, which characterizes external perturbations of some reference system. Such a Hamiltonian can be considered as a function of this parameter, that is, $H = H(h)$. In general, this implies that the eigenvalues and eigenvectors will be functions of h as well. In such cases, a possible scenario is to prepare the system initially in the ground state of the Hamiltonian $H(h_0)$, but then, suddenly change the parameter from h_0 to some other value h_1. The evolution in time of the initial state is then governed by the Hamiltonian $H(h_1)$. This process of abruptly changing the parameter h is called a sudden quench.

For a fixed value of the interaction coupling between the spins, g, the Hamiltonian of the transverse Ising chain in (2.4) may be viewed as a function of the external field, h. Namely, we will take the system to be initially in the ground state represented by $\Omega(h_0)$ for some initial external field, h_0. We consider the evolution in time for some other external field, h_1. Explicitly, the evolution in time is given by

$$\Psi(t, h_1, h_0) = \exp\left(-\mathrm{i}tH(h_1)\right)\Omega(h_0)\,. \tag{4.1}$$

We will call the state represented by this vector the quenched state.

Our goal in this section is to derive an expression for the order parameter correlation function with respect to the quenched state. That is, we will consider

$$\langle \Psi(t, h_1, h_0) | X_j X_k \Psi(t, h_1, h_0)\rangle\ ,$$

which we will call the quenched ground state correlation function from now on. We will find that the quenched ground state correlation function can be expressed as the Pfaffian of a certain antisymmetric matrix. The structure of this matrix will allow us to reduce the Pfaffian to a determinant. This determinant will be used to perform numerical calculations of the quenched ground state correlation function for a chain of finite size.

Expressions for the order parameter correlation function with respect to the quenched state in the thermodynamic limit have been determined by Pasquale Calabrese, Fabian Essler, and Maurizio Fagotti in [Calabrese et al., 2012a,b]. They found in [Calabrese et al., 2012b] that the quenched ground state correlation function approaches stationary values which are given by a generalized Gibbs ensemble. We will show this as well by using a stationary phase argument. In [Calabrese et al., 2012a], they provide expressions for the time-dependence of the quenched ground state correlation function for sufficiently large values of the time after the quench and the distance on the lattice. These results will be compared to our numerical calculations and we will conjecture an improved expression for the quenched ground state correlator in the case of quenches within the paramagnetic phase.

For the rest of this chapter, we will restrict the values of the spin interaction coupling, g, the initial external field, h_0, and the final external field, h_1, to be positive. Further, we will denote with h a generic positive value for the external field.

4.1 Quenched Ground State Correlation Function

We begin by considering a system of finite size, N. We argued in Section 2.5 that, for finite system sizes, the ground state of the Hamiltonian of the transverse Ising chain is given by the ground state of the even part of the Hamiltonian as long as g and h are positive. Therefore, for any value $h > 0$ of the external field, if $\Omega(h)$ represents the ground state of $H(h)$ and if $\tilde{\Omega}(h)$ represents the ground state of $H_P(h)$, then we can set $\Omega(h) = \tilde{\Omega}(h)$. In addition, $\tilde{\Omega}(h)$ represents the vacuum state of the fermionic Bogoliubov operators, $c_p(h)$, for momentum values $p \in P_N$. These facts enabled us in Chapter 3 to use Wick's theorem in order to determine the correlation functions of the Pauli operators with respect to the ground state of the transverse Ising chain. Subsequently, we will show that an analogous reasoning allows us to determine the quenched ground state correlation function for finite system sizes.

Let us consider the time evolution of the initial ground state, which is represented by $\Omega(h_0)$, induced by an Hamiltonian $H(h)$. We derived in Section 2.2 that the Hamiltonian is given by the orthogonal sum of two Hermitian operators which mutually commute. Namely, we have that $H(h) = H_P(h)P + H_Q(h)Q$, where $H_P(h)P$ and $H_Q(h)Q$ are orthogonal and commute. Since $\Omega(h_0) = \tilde{\Omega}(h_0)$ and since $\tilde{\Omega}(h_0)$ is in the even subspace, $P(\mathcal{H}_N)$, as we found in Section 2.5, we obtain for the time evolution of the initial ground state that

$$\begin{aligned}\exp\left(-\mathrm{i}tH(h)\right)\Omega(h_0) &= \exp\left(-\mathrm{i}tH_P(h)P\right)\exp\left(-\mathrm{i}tH_Q(h)Q\right)\Omega(h_0)\\ &= \exp\left(-\mathrm{i}tH_P(h)\right)\Omega(h_0)\,.\end{aligned}$$

That is, the time evolution of the ground state is governed only by the even part of the Hamiltonian, which has the form of a fermionic quantum harmonic oscillator in terms of the Bogoliubov operators, $c_p(h)$, where $p \in P_N$, as we have found in (2.84).

By defining the unitary time evolution operator

$$U(t,h) \coloneqq \exp\left(-\mathrm{i}tH_P(h)\right) , \tag{4.2}$$

we can write the time evolution of the initial ground state more compactly as $U(t,h)\Omega(h_0)$. In particular, the quenched state is represented by $\Psi(t,h_1,h_0) = U(t,h_1)\Omega(h_0)$.

By using the time evolution operator, we can rewrite the quenched ground state correlation function as

$$\langle \Psi(t,h_1,h_0) | X_j X_k \Psi(t,h_1,h_0) \rangle = \left\langle \Omega(h_0) \middle| U^\dagger(t,h_1) X_j X_k U(t,h_1) \Omega(h_0) \right\rangle , \tag{4.3}$$

for any $j,k \in \{0,1,\ldots,N-1\}$. This expression indicates that if we were able to rewrite $U^\dagger(t,h)X_jX_kU(t,h)$ as a product of mutually anticommuting operators, then we could use Wick's theorem and express the quenched ground state correlator as a Pfaffian. That is to say, we could use the same techniques which we employed in Section 3.1.

To this end, we define the operators

$$\bar{A}_j(t,h) \coloneqq U^\dagger(t,h) A_j U(t,h) , \tag{4.4}$$
$$\bar{B}_j(t,h) \coloneqq U^\dagger(t,h) B_j U(t,h) , \tag{4.5}$$

for all $j \in \{0,1,\ldots,N-1\}$, where A_j and B_j are given in (2.22) and (2.23). Since $U(t,h)$ is unitary and since all possible anticommutators of A_j and B_j, which are given in (2.24), (2.25), and (2.26), are proportional to the identity operator, we obtain that

$$\bar{A}_j(t,h)\bar{A}_k(t,h) + \bar{A}_k(t,h)\bar{A}_j(t,h) = 2\delta_{jk} , \tag{4.6}$$
$$\bar{B}_j(t,h)\bar{B}_k(t,h) + \bar{B}_k(t,h)\bar{B}_j(t,h) = -2\delta_{jk} , \tag{4.7}$$
$$\bar{A}_j(t,h)\bar{B}_k(t,h) + \bar{B}_k(t,h)\bar{A}_j(t,h) = 0 , \tag{4.8}$$

for any $j,k \in \{0,1,\ldots,N-1\}$.

We only need to consider $U^\dagger(t,h)X_jX_kU(t,h)$ for such $j,k \in \{0,1,\ldots,N-1\}$ for which $j<k$. This is no loss of generality for the same reasons we have already discussed in Section 3.1. Namely, for $j=k$ the products reduce to squares of the Pauli operators, which are the identity operator. For $j>k$, we can commute the Pauli operators and interchange the labels j and k. Thus, let $j,k \in \{0,1,\ldots,N-1\}$ such that $j<k$. In Section 3.1, we expressed the operators X_jX_k as products of the operators A_l and B_l, with the result being (3.3). We can use that identity to rewrite the transformed operators $U^\dagger(t,h)X_jX_kU(t,h)$ as products of the newly defined

operators $\bar{A}_l(t,h)$ and $\bar{B}_l(t,h)$. Namely, we insert the identity operator in the form of $I = U^\dagger(t,h)U(t,h)$ in between the operators A_l and B_l in expression (3.3). This leads to

$$U^\dagger(t,h)X_jX_kU(t,h) = (-1)^{r(r-1)/2}\bar{B}_j(t,h)\bar{B}_{j+1}(t,h)\cdots\bar{B}_{k-1}(t,h) \\ \bar{A}_{j+1}(t,h)\bar{A}_{j+2}(t,h)\cdots\bar{A}_k(t,h)\,. \quad (4.9)$$

Using the anticommutation relations of the $\bar{A}_l(t,h)$ and $\bar{B}_l(t,h)$ operators, we realize that all the operators in the product mutually anticommute. Moreover, this expression is similar to (3.3) since we only need to exchange the A_l and B_l in (3.3) with their time-propagated versions $\bar{A}_l(t,h)$ and $\bar{B}_l(t,h)$, respectively, in order to obtain the above result. Therefore, we are formally in the same position as we were in Section 3.1. That is to say that we can employ Wick's theorem to express the quenched ground state correlator in terms of two-point functions, which will ultimately lead to a Pfaffian, resembling the formula (3.12).

For $j,k \in \{0,1,\ldots,N-1\}$, we define the expressions

$$\bar{G}_{jk}(t,h_1,h_0) := \left\langle \Omega(h_0) \middle| \bar{B}_j(t,h_1)\bar{A}_k(t,h_1)\Omega(h_0) \right\rangle\,, \quad (4.10)$$

$$\bar{Q}_{jk}(t,h_1,h_0) := \left\langle \Omega(h_0) \middle| \bar{A}_j(t,h_1)\bar{A}_k(t,h_1)\Omega(h_0) \right\rangle\,, \quad (4.11)$$

$$\bar{S}_{jk}(t,h_1,h_0) := \left\langle \Omega(h_0) \middle| \bar{B}_j(t,h_1)\bar{B}_k(t,h_1)\Omega(h_0) \right\rangle\,. \quad (4.12)$$

Since we have periodic boundary conditions, the system is translationally invariant and, therefore, we have that

$$\bar{G}_{jk}(t,h_1,h_0) = \bar{g}_{k-j}(t,h_1,h_0)\,, \quad (4.13)$$

$$\bar{Q}_{jk}(t,h_1,h_0) = \bar{q}_{k-j}(t,h_1,h_0)\,, \quad (4.14)$$

$$\bar{S}_{jk}(t,h_1,h_0) = \bar{s}_{k-j}(t,h_1,h_0) \quad (4.15)$$

for some functions $\bar{g}_m$, $\bar{q}_m$, and $\bar{s}_m$, with $m \in \mathbb{Z}$, which are yet to be determined. For the sake of brevity and simplicity, we will suppress the arguments of these functions from now on, whenever there is no risk of misconception.

For any $r \in \{1,2,\ldots,N-1\}$, by using (3.1), we obtain for the quenched ground state correlation function that

$$\langle\Psi|X_0X_r\Psi\rangle = (-1)^{r(r-1)/2}\,\mathrm{pf}\begin{bmatrix} 0 & \bar{s}_1 & \bar{s}_2 & \cdots & \bar{s}_{r-1} & \bar{g}_1 & \bar{g}_2 & \cdots & \bar{g}_r \\ & 0 & \bar{s}_1 & \cdots & \bar{s}_{r-2} & \bar{g}_0 & \bar{g}_1 & \cdots & \bar{g}_{r-1} \\ & & \ddots & \ddots & \vdots & \vdots & \vdots & & \vdots \\ & & & 0 & \bar{s}_1 & \bar{g}_{-r+3} & \bar{g}_{-r+4} & \cdots & \bar{g}_2 \\ & & & & 0 & \bar{g}_{-r+2} & \bar{g}_{-r+3} & \cdots & \bar{g}_1 \\ & & & & & 0 & \bar{q}_1 & \cdots & \bar{q}_{r-1} \\ & & & & & & \ddots & \ddots & \vdots \\ & & & & & & & 0 & \bar{q}_1 \\ & & & & & & & & 0 \end{bmatrix}, \tag{4.16}$$

where the lower triangular part of the matrix is the negative of the transpose of the upper triangular part. All that remains is to determine the functions $\bar{g}_m$, $\bar{q}_m$, and $\bar{s}_m$ in order to be able to calculate the quenched ground state correlation function. For this purpose, we need to first determine $\bar{G}_{jk}$, $\bar{Q}_{jk}$, and $\bar{S}_{jk}$ for any $j,k \in \{0,1,\ldots,N-1\}$ and, then, derive appropriate expressions for $\bar{g}_m$, $\bar{q}_m$, and $\bar{s}_m$ by using the identities in (4.13), (4.14), and (4.15).

Let $j \in \{0,1,\ldots,N-1\}$ and define

$$\bar{a}_j(t,h) \coloneqq U^\dagger(t,h)a_jU(t,h)\,. \tag{4.17}$$

By substituting this operator into the defintions of $\bar{A}_j(t,h)$ and $\bar{B}_j(t,h)$, we obtain that

$$\bar{A}_j(t,h) = \bar{a}_j^\dagger(t,h) + \bar{a}_j(t,h)\,, \tag{4.18}$$

$$\bar{B}_j(t,h) = \bar{a}_j^\dagger(t,h) - \bar{a}_j(t,h)\,. \tag{4.19}$$

If we substitute the inversion of the Fourier transformation, which is given in (2.54), into the definition of $\bar{a}_j(t,h)$, we find that

$$\bar{a}_j(t,h) = \frac{1}{\sqrt{N}}\sum_{p\in P_N} U^\dagger(t,h)b_pU(t,h)e^{\mathrm{i}pj}\,. \tag{4.20}$$

Therefore, we need to express $U^\dagger(t,h)b_pU(t,h)$ for any $p \in P_N$ in terms of the initial Bogoliubov operators $c_q(h_0)$ and $c_q^\dagger(h_0)$ with $q \in P_N$.

Let $p \in \frac{\pi}{N}\mathbb{Z}$. In Section 2.4, we determined functions $u_p(h)$ and $v_p(h)$ such that

$$\begin{bmatrix} c_p(h) \\ c_{-p}^\dagger(h)\end{bmatrix} = \begin{bmatrix} u_p(h) & v_p(h) \\ v_p(h) & u_p(h)\end{bmatrix}\begin{bmatrix} b_p \\ b_{-p}^\dagger\end{bmatrix}, \tag{4.21}$$

The properties of the functions $u_p(h)$ and $v_p(h)$, which are given in the aforementioned section, ensured that the matrix is unitary, which is why we can invert this equation and obtain that

$$\begin{bmatrix} b_p \\ b^\dagger_{-p} \end{bmatrix} = \begin{bmatrix} u^*_p(h) & v^*_p(h) \\ v^*_p(h) & u^*_p(h) \end{bmatrix} \begin{bmatrix} c_p(h) \\ c^\dagger_{-p}(h) \end{bmatrix} . \tag{4.22}$$

Additionally, due to (2.84) and (4.2), we have that

$$U^\dagger(t,h)c_p(h)U(t,h) = e^{-\mathrm{i}t\omega_p(h)}c_p(h) . \tag{4.23}$$

By using these identities, we obtain that

$$\begin{bmatrix} U^\dagger(t,h)b_pU(t,h) \\ U^\dagger(t,h)b^\dagger_{-p}U(t,h) \end{bmatrix} = \begin{bmatrix} u^*_p(h) & v^*_p(h) \\ v^*_p(h) & u^*_p(h) \end{bmatrix} \begin{bmatrix} e^{-\mathrm{i}t\omega_p(h)} & 0 \\ 0 & e^{\mathrm{i}t\omega_p(h)} \end{bmatrix}$$
$$\begin{bmatrix} u_p(h) & v_p(h) \\ v_p(h) & u_p(h) \end{bmatrix} \begin{bmatrix} u^*_p(h_0) & v^*_p(h_0) \\ v^*_p(h_0) & u^*_p(h_0) \end{bmatrix} \begin{bmatrix} c_p(h_0) \\ c^\dagger_{-p}(h_0) \end{bmatrix}$$

We only need to determine the entries of the product of these matrices in the first row since we are only interested in $U^\dagger(t,h)b_pU(t,h)$ and since the ones in the second row are related to the ones in the first row by the canonical anticommutation relations, which are satisfied by both the Fourier transformed Jordan-Wigner operators and by the Bogoliubov operators. Let $\bar{u}^*_p(t,h,h_0)$ denote the entry in the first row and the first column and let $\bar{v}^*_p(t,h,h_0)$ denote the entry in the first row and the second column. These functions are given by

$$\begin{aligned} \bar{u}_p(t,h,h_0) = &\left(|u_p(h)|^2e^{\mathrm{i}\omega_p(h)t} + |v_p(h)|^2e^{-\mathrm{i}\omega_p(h)t}\right)u_p(h_0) \\ &+ \left(u_p(h)v^*_p(h)e^{\mathrm{i}\omega_p(h)t} + u^*_p(h)v_p(h)e^{-\mathrm{i}\omega_p(h)t}\right)v_p(h_0) , \end{aligned} \tag{4.24}$$

and

$$\begin{aligned} \bar{v}_p(t,h,h_0) = &\left(|u_p(h)|^2e^{\mathrm{i}\omega_p(h)t} + |v_p(h)|^2e^{-\mathrm{i}\omega_p(h)t}\right)v_p(h_0) \\ &+ \left(u_p(h)v^*_p(h)e^{\mathrm{i}\omega_p(h)t} + u^*_p(h)v_p(h)e^{-\mathrm{i}\omega_p(h)t}\right)u_p(h_0) . \end{aligned} \tag{4.25}$$

We extend their definition from $p \in \frac{\pi}{N}\mathbb{Z}$ to all $p \in \mathbb{R}$ by using these identities. For the operator $U^\dagger(t,h)b_pU(t,h)$, we have that

$$U^\dagger(t,h)b_pU(t,h) = \bar{u}^*_p(t,h,h_0)c_p(h_0) + \bar{v}^*_p(t,h,h_0)c^\dagger_{-p}(h_0) . \tag{4.26}$$

Substitution of this identity into (4.20) gives that

$$\bar{a}_j(t,h) = \frac{1}{\sqrt{N}} \sum_{p\in P_N} \left(\bar{u}_p(t,h,h_0)c_p(h_0) + \bar{v}_p(t,h,h_0)c^\dagger_{-p}(h_0)\right)e^{\mathrm{i}pj} \tag{4.27}$$

for all $j \in \{0, 1, \ldots, N-1\}$. Introducing the expressions

$$\bar{u}_{pj}(t, h, h_0) := \frac{1}{\sqrt{N}} \bar{u}_p^*(t, h, h_0) e^{-\mathrm{i}pj} , \tag{4.28}$$

$$\bar{v}_{pj}(t, h, h_0) := \frac{1}{\sqrt{N}} \bar{v}_{-p}(t, h, h_0) e^{-\mathrm{i}pj} , \tag{4.29}$$

we obtain that

$$\bar{a}_j(t, h) = \sum_{p \in P_N} \Big(\bar{u}_{pj}^*(t, h, h_0) c_p(h_0) + \bar{v}_{pj}(t, h, h_0) c_p^\dagger(h_0) \Big) . \tag{4.30}$$

Let $j, k \in \{0, 1, \ldots, N-1\}$. Equation (4.30) is formally analogous to the expression given in (3.15). Since only the initial Bogoliubov operators appear in (4.30), we obtain by the same reasoning as in Section 3.1 that

$$\bar{G}_{jk} = \sum_{p \in P_N} (\bar{v}_{pj}^* - \bar{u}_{pj}^*)(\bar{u}_{pk} + \bar{v}_{pk}) , \tag{4.31}$$

$$\bar{Q}_{jk} = \sum_{p \in P_N} (\bar{v}_{pj}^* + \bar{u}_{pj}^*)(\bar{u}_{pk} + \bar{v}_{pk}) , \tag{4.32}$$

$$\bar{S}_{jk} = \sum_{p \in P_N} (\bar{v}_{pj}^* - \bar{u}_{pj}^*)(\bar{u}_{pk} - \bar{v}_{pk}) . \tag{4.33}$$

Substituting the definitions of $\bar{u}_{pj}$ and $\bar{v}_{pj}$, we obtain that

$$\bar{G}_{jk} = -\frac{1}{N} \sum_{p \in P_N} \Big(|\bar{u}_p|^2 - |\bar{v}_{-p}|^2 - 2\mathrm{i}\,\mathrm{Im}(\bar{u}_p \bar{v}_{-p}) \Big)\, e^{-\mathrm{i}p(k-j)} , \tag{4.34}$$

$$\bar{Q}_{jk} = +\frac{1}{N} \sum_{p \in P_N} \Big(|\bar{u}_p|^2 + |\bar{v}_{-p}|^2 + 2\,\mathrm{Re}(\bar{u}_p \bar{v}_{-p}) \Big)\, e^{-\mathrm{i}p(k-j)} , \tag{4.35}$$

$$\bar{S}_{jk} = -\frac{1}{N} \sum_{p \in P_N} \Big(|\bar{u}_p|^2 + |\bar{v}_{-p}|^2 - 2\,\mathrm{Re}(\bar{u}_p \bar{v}_{-p}) \Big)\, e^{-\mathrm{i}p(k-j)} . \tag{4.36}$$

These identities allow us to identify $\bar{g}_m$, $\bar{q}_m$, and $\bar{s}_m$ by using the equations (4.13), (4.14), and (4.15). Namely, for any $m \in \mathbb{Z}$, we see that

$$\bar{g}_m = -\frac{1}{N} \sum_{p \in P_N} \Big(|\bar{u}_p|^2 - |\bar{v}_{-p}|^2 - 2\mathrm{i}\,\mathrm{Im}(\bar{u}_p \bar{v}_{-p}) \Big)\, e^{-\mathrm{i}pm} , \tag{4.37}$$

$$\bar{q}_m = +\frac{1}{N} \sum_{p \in P_N} \Big(|\bar{u}_p|^2 + |\bar{v}_{-p}|^2 + 2\,\mathrm{Re}(\bar{u}_p \bar{v}_{-p}) \Big)\, e^{-\mathrm{i}pm} , \tag{4.38}$$

$$\bar{s}_m = -\frac{1}{N} \sum_{p \in P_N} \Big(|\bar{u}_p|^2 + |\bar{v}_{-p}|^2 - 2\,\mathrm{Re}(\bar{u}_p \bar{v}_{-p}) \Big)\, e^{-\mathrm{i}pm} . \tag{4.39}$$

In order to simplify the expressions for $\bar{g}_m$, $\bar{q}_m$, and $\bar{s}_m$, we need to consider

$\bar{u}_p(t,h,h_0)$ and $\bar{v}_p(t,h,h_0)$ in more detail. Let $p \in \mathbb{R}$ with $p \notin \pi\mathbb{Z}$. Then, we find that

$$\bar{u}_p(t,h,h_0) = \cos(\omega_p(h)t)u_p(h_0) + \mathrm{i}(\alpha_p(h)u_p(h_0) - \beta_p(h)v_p(h_0))\frac{\sin(\omega_p(h)t)}{\omega_p(h)}\,, \quad (4.40)$$

$$\bar{v}_p(t,h,h_0) = \cos(\omega_p(h)t)v_p(h_0) + \mathrm{i}(\alpha_p(h)v_p(h_0) - \beta_p(h)u_p(h_0))\frac{\sin(\omega_p(h)t)}{\omega_p(h)}\,. \quad (4.41)$$

For $p \in 2\pi\mathbb{Z}$, we have that

$$\bar{u}_p(t,h,h_0) = \begin{cases} e^{\mathrm{i}t\omega_p(h)} & \text{if } h \geq g \text{ and } h_0 \geq g, \\ e^{-\mathrm{i}t\omega_p(h)} & \text{if } h < g \text{ and } h_0 \geq g, \\ 0 & \text{otherwise,} \end{cases} \quad (4.42)$$

$$\bar{v}_p(t,h,h_0) = \begin{cases} -\mathrm{i}e^{\mathrm{i}t\omega_p(h)} & \text{if } h \geq g \text{ and } h_0 < g, \\ -\mathrm{i}e^{-\mathrm{i}t\omega_p(h)} & \text{if } h < g \text{ and } h_0 < g, \\ 0 & \text{otherwise.} \end{cases} \quad (4.43)$$

For $p \in \pi\mathbb{Z}$, we have that

$$\bar{u}_p(t,h,h_0) = \begin{cases} e^{\mathrm{i}t\omega_p(h)} & \text{if } h \geq -g \text{ and } h_0 \geq -g, \\ e^{-\mathrm{i}t\omega_p(h)} & \text{if } h < -g \text{ and } h_0 \geq -g, \\ 0 & \text{otherwise,} \end{cases} \quad (4.44)$$

$$\bar{v}_p(t,h,h_0) = \begin{cases} -\mathrm{i}e^{\mathrm{i}t\omega_p(h)} & \text{if } h \geq -g \text{ and } h_0 < -g, \\ -\mathrm{i}e^{-\mathrm{i}t\omega_p(h)} & \text{if } h < -g \text{ and } h_0 < -g, \\ 0 & \text{otherwise.} \end{cases} \quad (4.45)$$

Using these identities, we find that $|\bar{v}_{-p}| = |\bar{v}_p|$. If $p \notin \pi\mathbb{Z}$, we even have that $\bar{v}_{-p} = -\bar{v}_p$. Furthermore, since the Fourier transformed Jordan-Wigner operators satisfy the canonical anticommutation relations, which are given in the (2.51) and (2.52), we have that $|\bar{u}_p|^2 + |\bar{v}_p|^2 = 1$.

Starting from the expressions (4.37), (4.38), and (4.39), we proceed as follows. We split the sum over the set P_N into a summation over the positive and into a summation over the negative summation indices. Then, we rewrite the sum over the negative indices as a sum over the positive ones and combine the terms where it is possible to combine them. This procedure will depend on the parity of N since if N is even, the set P_N consists fully of pairs of positive and corresponding negative values, whereas if N is odd, there is one element in P_N, namely $-\pi$, which does not have a corresponding positive part in the set. This can be seen in the definition of P_N given in (2.53). However, performing the described procedure, we observe that the parity of N only makes a difference for $\bar{g}_m$. The expressions $\bar{q}_m$ and $\bar{s}_m$ do not depend on the parity of N. Explicitly, we obtain that

$$\bar{g}_m = \delta_{m=0 \bmod N} - \frac{4}{N} \sum_{p \in P_N^+} \Big(|\bar{u}_p|^2 \cos(pm) + \mathrm{Im}(\bar{u}_p \bar{v}_p) \sin(pm) \Big) \,, \tag{4.46}$$

if N is even, and

$$\bar{g}_m = -\frac{(-1)^m}{N} + \delta_{m=0 \bmod N} - \frac{4}{N} \sum_{p \in P_N^+} \Big(|\bar{u}_p|^2 \cos(pm) + \mathrm{Im}(\bar{u}_p \bar{v}_p) \sin(pm) \Big) \,, \tag{4.47}$$

if N is odd. For $\bar{q}_m$ and $\bar{s}_m$, we obtain, independent of the parity of N, that

$$\bar{q}_m = +\delta_{m=0 \bmod N} + \frac{4\mathrm{i}}{N} \sum_{p \in P_N^+} \mathrm{Re}(\bar{u}_p \bar{v}_p) \sin(pm) \,, \tag{4.48}$$

$$\bar{s}_m = -\delta_{m=0 \bmod N} + \frac{4\mathrm{i}}{N} \sum_{p \in P_N^+} \mathrm{Re}(\bar{u}_p \bar{v}_p) \sin(pm) \,. \tag{4.49}$$

In [Calabrese et al., 2012a], the authors managed to reduce the Pfaffian given in (4.16) to the determinant of a Toeplitz plus Hankel matrix. They used the eigenvalues of a certain block Toeplitz matrix (which can be obtained from the matrix in (4.16) by permuting rows and corresponding columns) to perform the reduction. In the following, we will present our own proof for this reduction, which involves only multiplication of matrices and basic properties of the determinant and the Pfaffian and, thus, is simpler. To this end, we observe that $\bar{s}_m = -\bar{q}_m^*$ for all $m \in \mathbb{Z}$. In particular, if m is not an integer multiple of N, then we even have that $\bar{s}_m = \bar{q}_m$. We can use this relation to simplify the Pfaffian.

For this purpose, let $r \in \{1, 2, \ldots, N-1\}$ and introduce the r by r Toeplitz matrices

$$\bar{G}_r \coloneqq \begin{bmatrix} \bar{g}_1 & \bar{g}_2 & \cdots & \bar{g}_r \\ \bar{g}_0 & \bar{g}_1 & \cdots & \bar{g}_{r-1} \\ \vdots & \vdots & & \vdots \\ \bar{g}_{-r+3} & \bar{g}_{-r+4} & \cdots & \bar{g}_2 \\ \bar{g}_{-r+2} & \bar{g}_{-r+3} & \cdots & \bar{g}_1 \end{bmatrix} , \tag{4.50}$$

and

$$\bar{Q}_r \coloneqq \begin{bmatrix} 0 & \bar{q}_1 & \bar{q}_2 & \cdots & \bar{q}_{r-1} \\ & 0 & \bar{q}_1 & \cdots & \bar{q}_{r-2} \\ & & \ddots & \ddots & \vdots \\ & & & 0 & \bar{q}_1 \\ & & & & 0 \end{bmatrix} , \tag{4.51}$$

where the lower triangular part of $\bar{Q}_r$ is given by the negative of the transpose of the upper triangular part and where we kept the arguments t, h_1 and h_0 implicit. Note that $\bar{Q}_r$ is antisymmetric, which means that $\bar{Q}_r^{\mathrm{T}} = -\bar{Q}_r$. We define the $2r$ by $2r$ matrix

$$D_r := \begin{bmatrix} \bar{Q}_r & \bar{G}_r \\ -\bar{G}_r^{\mathrm{T}} & \bar{Q}_r \end{bmatrix} . \tag{4.52}$$

Then, we can rewrite expression (4.16) in the form

$$\langle \Psi(t,h_1,h_0) | X_0 X_r \Psi(t,h_1,h_0) \rangle = (-1)^{r(r-1)/2} \operatorname{pf} D_r(t,h_1,h_0) . \tag{4.53}$$

For a positive integer n, let F_n denote the n by n flip matrix, which is given by $(F_n)_{jk} = \delta_{j,n-1-k}$ for all $j,k \in \{0,1,\dots,n-1\}$. That is, F_n is the n by n matrix which has ones on the antidiagonal and zero for all other entries. If M denotes an arbitrary n by n matrix, then the matrix MF_n is the one obtained from M by reversing the order of its columns and $F_n M$ is the one obtained from M by reversing the order of its rows. In particular, if T denotes an n by n Toeplitz matrix, then $F_n T F_n = T^{\mathrm{T}}$. This implies that $F_r \bar{G}_r F_r = \bar{G}_r^{\mathrm{T}}$ and that $F_r \bar{Q}_r F_r = \bar{Q}_r^{\mathrm{T}} = -\bar{Q}_r$.

We define the $2r$ by $2r$ matrix

$$S_r := \frac{1}{\sqrt{2}} \begin{bmatrix} I_r & F_r \\ F_r & -I_r \end{bmatrix} , \tag{4.54}$$

where I_r denotes the r by r identity matrix. Then, we obtain that

$$\begin{aligned} S_r D_r S_r^{\mathrm{T}} &= \frac{1}{2} \begin{bmatrix} I_r & F_r \\ F_r & -I_r \end{bmatrix} \begin{bmatrix} \bar{Q}_r & \bar{G}_r \\ -\bar{G}_r^{\mathrm{T}} & \bar{Q}_r \end{bmatrix} \begin{bmatrix} I_r & F_r \\ F_r & -I_r \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} \bar{Q}_r - F_r \bar{G}_r^{\mathrm{T}} + \bar{G}_r F_r + F_r \bar{Q}_r F_r & \bar{Q}_r F_r - F_r \bar{G}_r^{\mathrm{T}} F_r - \bar{G}_r - F_r \bar{Q}_r \\ F_r \bar{Q}_r + \bar{G}_r^{\mathrm{T}} + F_r \bar{G}_r F_r - \bar{Q}_r F_r & F_r \bar{Q}_r F_r + \bar{G}_r^{\mathrm{T}} F_r - F_r \bar{G}_r + \bar{Q}_r \end{bmatrix} \\ &= \begin{bmatrix} 0 & \bar{Q}_r F_r - \bar{G}_r \\ F_r \bar{Q}_r + \bar{G}_r^{\mathrm{T}} & 0 \end{bmatrix} \\ &= \begin{bmatrix} 0 & \bar{Q}_r F_r - \bar{G}_r \\ -(\bar{Q}_r F_r - \bar{G}_r)^{\mathrm{T}} & 0 \end{bmatrix} . \end{aligned}$$

Furthermore, we have that

$$\det S_r = \det \frac{1}{\sqrt{2}} \begin{bmatrix} I_r & F_r \\ F_r & -I_r \end{bmatrix} = \det \left(-\frac{1}{2} I_r - \frac{1}{2} F_r^2 \right) = \det(-I_r) = (-1)^r .$$

Therefore, we obtain that

$$\operatorname{pf}(S_r D_r S_r^{\mathrm{T}}) = \det S_r \operatorname{pf} D_r = (-1)^r \operatorname{pf} D_r ,$$

and that

$$\mathrm{pf}(S_r D_r S_r^{\mathrm{T}}) = \mathrm{pf}\begin{bmatrix} 0 & \bar{Q}_r F_r - \bar{G}_r \\ -(\bar{Q}_r F_r - \bar{G}_r)^{\mathrm{T}} & 0 \end{bmatrix} = (-1)^{r(r-1)/2} \det(\bar{Q}_r F_r - \bar{G}_r)\,.$$

Eventually, putting everything together, we obtain the final result for the correlation function,

$$\langle \Psi(t,h_1,h_0) | X_0 X_r \Psi(t,h_1,h_0)\rangle = (-1)^r \det\Big(\bar{Q}_r(t,h_1,h_0)F_r - \bar{G}_r(t,h_1,h_0)\Big)\,, \tag{4.55}$$

for any $r \in \{1,\dots,N-1\}$. We will use this formula to numerically determine the correlation function on finite chains. This expression in terms of the determinant is more suited for calculations than the expression in terms of the Pfaffian since there are software packages which can evaluate the determinant efficiently.

4.2 Large Time Asymptotics

At this point, let us describe the thermodynamic limit. We argued in the preceding section that the time evolution operator leaves the even and odd subspaces invariant. More specifically, for any finite chain, we have that

$$\exp(-\mathrm{i}tH(h))\tilde{\Omega}(h_0) = \exp(-\mathrm{i}tH_P(h))\tilde{\Omega}(h_0)\,, \tag{4.56}$$

$$\exp(-\mathrm{i}tH(h))\hat{\Omega}(h_0) = \exp(-\mathrm{i}tH_Q(h))\hat{\Omega}(h_0)\,, \tag{4.57}$$

and since we saw in Section 2.2 that $H_P(h)$ and $H_Q(h)$ commute with the projectors P and Q, we find that $\exp(-\mathrm{i}tH(h))\tilde{\Omega}(h_0) \in P(\mathcal{H}_N)$ and that $\exp(-\mathrm{i}tH(h))\hat{\Omega}(h_0) \in Q(\mathcal{H}_N)$. This, in turn, implies that the situation here is similar to the situation in Section 3.2, where we determined the thermodynamic limit of the order parameter correlation function with respect to the ground state of the transverse Ising chain. This can be seen as follows: For $0 < h_0 < g$, we need to calculate the correlation function of the order parameter with respect to the state represented by $\exp(-\mathrm{i}tH(h))(\alpha\tilde{\Omega}(h_0)+\beta\hat{\Omega}(h_0))$ with $|\alpha|^2+|\beta|^2 = 1$ and, then, take the limit $N \to \infty$. The vectors $\exp(-\mathrm{i}tH(h))\tilde{\Omega}(h_0)$ and $X_0X_r\exp(-\mathrm{i}tH(h))\hat{\Omega}(h_0)$ as well as the vectors $\exp(-\mathrm{i}tH(h))\hat{\Omega}(h_0)$ and $X_0X_r\exp(-\mathrm{i}tH(h))\tilde{\Omega}(h_0)$ are mutually orthogonal since X_0X_r flips spins at two sites and, thus, leaves the subspaces $P(\mathcal{H}_N)$ and $Q(\mathcal{H}_N)$ invariant. The order parameter correlation function with respect to $\exp(-\mathrm{i}tH(h))\hat{\Omega}(h_0)$ differs from the one with respect to $\exp(-\mathrm{i}tH(h))\tilde{\Omega}(h_0)$, calculated in the previous section, by that the sums over the momenta in (4.37), (4.38), and (4.39) need to be taken over Q_N, given in (2.59). However, the sums over P_N and Q_N are the Riemann sums of the integrals of the same respective functions. Therefore, the limits of the order parameter correlation function with respect to $\exp(-\mathrm{i}tH(h))\tilde{\Omega}(h_0)$ and with respect to $\exp(-\mathrm{i}tH(h))\hat{\Omega}(h_0)$ as $N \to \infty$ are the same. That is to say that we can simply take the limit $N \to \infty$ of the expression (4.55) to obtain the order parameter correlation function with respect to the quenched state in the thermodynamic limit.

Our aim is to determine the behaviour of the quenched ground state correlation function in the thermodynamic limit for asymptotically large times, $t \gg g^{-1}$. To this end, we need to determine the thermodynamic limit of the quenched ground state correlation function, which we denote by $\bar{C}_r$, first. We already realized that it suffices to take the limit $N \to \infty$ of the expression (4.55). Since the determinant is a continuous function of the entries of the matrix, this amounts to taking the limit $N \to \infty$ of (4.37) and (4.38).

In order to consider the limit $N \to \infty$, let us make the dependencies on N explicit. We introduce

$$\bar{g}_{N,m} \coloneqq -\frac{1}{N} \sum_{p \in P_N} \Big(|\bar{u}_p|^2 - |\bar{v}_{-p}|^2 - 2\mathrm{i}\,\mathrm{Im}(\bar{u}_p \bar{v}_{-p}) \Big)\, e^{-\mathrm{i}pm}\,, \tag{4.58}$$

$$\bar{q}_{N,m} \coloneqq +\frac{1}{N} \sum_{p \in P_N} \Big(|\bar{u}_p|^2 + |\bar{v}_{-p}|^2 + 2\,\mathrm{Re}(\bar{u}_p \bar{v}_{-p}) \Big)\, e^{-\mathrm{i}pm}\,, \tag{4.59}$$

for all $m \in \mathbb{Z}$. For a fixed $m \in \mathbb{Z}$, $\bar{g}_{N,m}(t, h_1, h_0)$ and $\bar{q}_{N,m}(t, h_1, h_0)$ are sequences in N. For any N, they are the Riemann sums of the integrals of the functions $[-\pi, \pi] \longrightarrow \mathbb{C}$ given by

$$p \mapsto \frac{-1}{2\pi} \Big(|\bar{u}_p(t, h_1, h_0)|^2 - |\bar{v}_{-p}(t, h_1, h_0)|^2 - 2\mathrm{i}\,\mathrm{Im}(\bar{u}_p(t, h_1, h_0)\bar{v}_{-p}(t, h_1, h_0)) \Big)\, e^{-\mathrm{i}pm}\,,$$
$$p \mapsto \frac{1}{2\pi} \Big(|\bar{u}_p(t, h_1, h_0)|^2 + |\bar{v}_{-p}(t, h_1, h_0)|^2 + 2\,\mathrm{Re}(\bar{u}_p(t, h_1, h_0)\bar{v}_{-p}(t, h_1, h_0)) \Big)\, e^{-\mathrm{i}pm}\,,$$

respectively. Therefore, $\bar{g}_{N,m}(t, h_1, h_0)$ and $\bar{q}_{N,m}(t, h_1, h_0)$ converge to the respective integrals of the above functions as $N \to \infty$. We denote these limits by $\bar{g}_m(t, h_1, h_0) = \lim_{N\to\infty} \bar{g}_{N,m}(t, h_1, h_0)$ and $\bar{q}_m(t, h_1, h_0) = \lim_{N\to\infty} \bar{q}_{N,m}(t, h_1, h_0)$.

To determine the limits $\bar{g}_m$ and $\bar{q}_m$ more explicitly, we restrict our calculations of $\bar{g}_{N,m}$ and $\bar{q}_{N,m}$ to even N since this case is easier to determine. This is justified since any subsequence of a convergent sequence converges to the same limit. For such even N, we obtain that

$$\bar{g}_{N,m} \coloneqq -\frac{1}{N} \sum_{p \in P_N} \Big(2|\bar{u}_p|^2 - 1 + 2\mathrm{i}\,\mathrm{Im}(\bar{u}_p \bar{v}_p) \Big)\, e^{-\mathrm{i}pm}\,, \tag{4.60}$$

$$\bar{q}_{N,m} \coloneqq +\frac{1}{N} \sum_{p \in P_N} \left(1 - 2\,\mathrm{Re}(\bar{u}_p \bar{v}_p)\right) e^{-\mathrm{i}pm}\,. \tag{4.61}$$

For any $p \in \mathbb{R}$ with $p \notin \pi\mathbb{Z}$, we have that

$$|\bar{u}_p(t,h,h_0)|^2 = \frac{1}{2} + \cos^2(\omega_p(h)t)\frac{\alpha_p(h_0)}{2\omega_p(h_0)} + \left(\left(\alpha_p^2(h) + \beta_p^2(h)\right)\frac{\alpha_p(h_0)}{2\omega_p(h_0)} - \alpha_p(h)\beta_p(h)\frac{\beta_p(h_0)}{\omega_p(h_0)}\right)\frac{\sin^2(\omega_p(h)t)}{\omega_p^2(h)}\,, \quad (4.62)$$

and that

$$\begin{aligned}\bar{u}_p(t,h,h_0)\bar{v}_p(t,h,h_0) &= \cos^2(\omega_p(h)t)\frac{\beta_p(h_0)}{2\omega_p(h_0)} + \mathrm{i}\frac{\sin(2t\omega_p(h))}{2\omega_p(h)}\frac{\alpha_p(h)\beta_p(h_0) - \beta_p(h)\alpha_p(h_0)}{\omega_p(h_0)} \\ &\quad - \left(\left(\alpha_p^2(h) + \beta_p^2(h)\right)\frac{\beta_p(h_0)}{2\omega_p(h_0)} - \alpha_p(h)\beta_p(h)\frac{\alpha_p(h_0)}{\omega_p(h_0)}\right)\frac{\sin^2(\omega_p(h)t)}{\omega_p^2(h)}\,. \quad (4.63)\end{aligned}$$

By substituting these expressions into $\bar{g}_{N,m}$ and $\bar{q}_{N,m}$ and taking the limit $N \to \infty$, we obtain

$$\begin{aligned}\bar{g}_m(t,h_1,h_0) &= -\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{(h_1h_0 - g(h_0+h_1)\cos p + g^2)(h_1 - ge^{\mathrm{i}p})}{(g^2+h_1^2-2gh_1\cos p)\sqrt{g^2+h_0^2-2gh_0\cos p}}e^{-\mathrm{i}pm}\mathrm{d}p \\ &\quad + \frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{i}g(h_0-h_1)\sin p(h_1-ge^{\mathrm{i}p})\cos(2t\omega_p(h_1))}{(g^2+h_1^2-2gh_1\cos p)\sqrt{g^2+h_0^2-2gh_0\cos p}}e^{-\mathrm{i}pm}\mathrm{d}p\,, \quad (4.64)\end{aligned}$$

and

$$\bar{q}_m(t,h_1,h_0) = \delta_{m0} + \frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{g(h_0-h_1)\sin p\sin(2t\omega_p(h_1))}{\sqrt{g^2+h_1^2-2gh_1\cos p}\sqrt{g^2+h_0^2-2gh_0\cos p}}e^{-\mathrm{i}pm}\mathrm{d}p\,. \quad (4.65)$$

Let us now consider the time-dependent parts of (4.64) and (4.65). Writing the cosine and sine functions in terms of the exponential function, we find that the time dependent parts take the generic form

$$I_\pm(t) := \int_{-\pi}^{\pi} f(p)e^{\pm 2\mathrm{i}t\omega_p}\,, \quad (4.66)$$

where f denotes some function which can be identified by comparing this expression to the functions multiplying the time-dependent terms in (4.64) and (4.65). We will use a stationary phase argument to extract $I_\pm(t)$ for asymptotically large t. The relevant theorems are taken from [Bhattacharya and Basu, 1979]. Namely, ω_p is stationary at the points $p=-\pi$, $p=0$, and $p=\pi$ within the closed intervall $[-\pi,\pi]$. In the cases at hand, the function f vanishes at all three points. However, the derivative f' does not vanish as long as we restrict ourselves to the cases where

$h_0 \neq g \neq h_1$ and $h_0 \neq h_1$. Therefore, the stationary phase formula gives that $I_\pm(t) \approx 0$ for asymptotically large t. This means that the time dependent parts in the above expressions vanish and we are left with

$$\bar{g}_m(t, h_1, h_0) \approx -\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{(h_1 h_0 - g(h_0 + h_1)\cos p + g^2)(h_1 - g e^{\mathrm{i}p})}{(g^2 + h_1^2 - 2gh_1 \cos p)\sqrt{g^2 + h_0^2 - 2gh_0 \cos p}} e^{-\mathrm{i}pm} \mathrm{d}p \,, \tag{4.67}$$

and that $\bar{q}_m(t, h_1, h_0) \approx \delta_{m0}$ for asymptotically large times t. Since the matrix $\bar{Q}_r$ in (4.55) does not involve $\bar{q}_m$ for $m = 0$, the expression for the quenched ground state correlation function in the thermodynamic limit reduces to $\bar{C}_r(t, h_1, h_0) \approx \det \bar{G}_r(t, h_1, h_0)$ for long times after the sudden quench. Therefore, the quenched ground state correlation function becomes independent of time, that is, it becomes stationary.

We will compare the result for the quenched ground state correlation function in the thermodynamic limit and for asymptotically large times with the corresponding correlation function obtained from a generalized Gibbs ensemble. Namely, consider an ensemble represented by the density operator

$$\varrho = \frac{1}{Z} \exp\left(-\sum_{p \in P_N} \beta_p \omega_p c_p^\dagger c_p \right) \,, \tag{4.68}$$

where Z is such that $\operatorname{tr} \varrho = 1$ and where β_p denote mode-dependent inverse temperatures from now on. The expectation value of an operator A with respect to this ensemble is given by $\langle A \rangle_{\mathrm{GGE}} = \operatorname{tr} \varrho A$. We are interested in the correlator $\langle X_j X_k \rangle_{\mathrm{GGE}}$ for $j, k \in \{0, 1, \ldots, N-1\}$ with $j < k$. For expectation values with respect to these kind of density operators, there is a theorem which corresponds to Wick's theorem in (3.1) (e.g., cf. [Nolting, 2009]). Therefore, we can express $\langle X_j X_k \rangle_{\mathrm{GGE}}$ as a Pfaffian of the two-point functions $\langle B_j A_k \rangle_{\mathrm{GGE}}$, $\langle A_j A_k \rangle_{\mathrm{GGE}}$, and $\langle B_j B_k \rangle_{\mathrm{GGE}}$. We obtain that

$$\langle B_j A_k \rangle_{\mathrm{GGE}} = -\frac{1}{N} \sum_{p \in P_N} \frac{h - g e^{\mathrm{i}p}}{\sqrt{g^2 + h^2 - 2gh\cos p}} \left(1 - 2 \left\langle c_p^\dagger c_p \right\rangle_{\mathrm{GGE}} \right) e^{-\mathrm{i}p(k-j)} \tag{4.69}$$

and that $\langle A_j A_k \rangle_{\mathrm{GGE}} = \delta_{jk} = -\langle B_j B_k \rangle_{\mathrm{GGE}}$. We fix the mode-dependent inverse temperatures by the condition

$$\left\langle c_p^\dagger(h_1) c_p(h_1) \right\rangle_{\mathrm{GGE}} = \left\langle \Psi(t, h_1, h_0) \middle| c_p^\dagger(h_1) c_p(h_1) \Psi(t, h_1, h_0) \right\rangle \,. \tag{4.70}$$

Since the quenched state is represented by $\Psi(t, h_1, h_0) = U(t, h_1)\Omega(h_0)$ and since we have that $U^\dagger(t, h_1) c_p(h_1) U(t, h_1) = e^{-\mathrm{i}t\omega_p(h_1)} c_p(h_1)$ for any $p \in P_N$, we find that

$$\left\langle \Psi(t, h_1, h_0) \middle| c_p^\dagger(h_1) c_p(h_1) \Psi(t, h_1, h_0) \right\rangle = \left\langle \Omega(h_0) \middle| c_p^\dagger(h_1) c_p(h_1) \Omega(h_0) \right\rangle \,, \tag{4.71}$$

for all $p, q \in P_N$. This means that the mode occupation numbers of the final Bogoliubov fermions with respect to the quenched state do not depend on the time passed after the sudden quench. We need to consider the expectation values of $c_p^\dagger(h)c_p(h)$ with respect to the initial ground state. Since $\Omega(h_0)$ represents the vacuum state of the initial Bogoliubov fermions, $c_p(h_0)$ with $p \in P_N$, the idea is to express $c_p(h)$ in terms of $c_p(h_0)$. This can be achieved by using the expressions (4.21) and (4.22). Let $p \in \frac{\pi}{N}\mathbb{Z}$. Then, we obtain that

$$\begin{bmatrix} c_p(h) \\ c_{-p}(h) \end{bmatrix} = \begin{bmatrix} u_p(h) & v_p(h) \\ v_p(h) & u_p(h) \end{bmatrix} \begin{bmatrix} u_p^*(h_0) & v_p^*(h_0) \\ v_p^*(h_0) & u_p^*(h_0) \end{bmatrix} \begin{bmatrix} c_p(h_0) \\ c_{-p}(h_0) \end{bmatrix} .$$

Therefore, we can write

$$c_p(h) = f_p(h, h_0)c_p(h_0) + g_p(h, h_0)c_{-p}^\dagger(h_0) , \tag{4.72}$$

where we used the functions given by

$$f_p(h, h_0) \coloneqq u_p(h)u_p^*(h_0) + v_p(h)v_p^*(h_0) , \tag{4.73}$$

$$g_p(h, h_0) \coloneqq u_p(h)v_p^*(h_0) + v_p(h)u_p^*(h_0) . \tag{4.74}$$

From this expression for $c_p(h)$, it follows that

$$\left\langle \Omega(h_0) \middle| c_k^\dagger(h_1)c_k(h_1)\Omega(h_0) \right\rangle = |g_p(h_1, h_0)|^2 , \tag{4.75}$$

for all $p \in P_N$. In particular, we have that $1-2\left\langle c_p(h_1)^\dagger c_p(h_1)\right\rangle_{\mathrm{GGE}} = 1-2|g_p(h_1, h_0)|^2$ since we have chosen the mode-dependent temperatures by $\left\langle c_p(h_1)^\dagger c_p(h_1)\right\rangle_{\mathrm{GGE}} = |g_p(h_1, h_0)|^2$. Evaluating $1 - 2|g_p(h_1, h_0)|^2$ gives that

$$1 - 2|g_p(h_1, h_0)|^2 = \frac{h_1 h_0 - g(h_0 + h_1)\cos p + g^2}{\sqrt{g^2 + h_1^2 - 2gh_1 \cos p}\sqrt{g^2 + h_0^2 - 2gh_0 \cos p}} .$$

If we substitute this expression into (4.69) and take the limit $N \to \infty$ of the result, we obtain the right hand side of (4.67). Therefore, the quenched ground state correlation function is given by the generealized Gibbs ensemble for asymptotically large values of the time after the quench.

In particular, we find that the quenched ground state correlation function is given by a determinant of a Toeplitz matrix for asymptotically large values of t. This suggest that the situation is analogous to the calculations performed in Section 3, where the ground state correlation function of the order parameter X_j was given by a determinant of a Toeplitz matrix as well. It turns out that it is possible to obtain expressions for the quenched correlation function after long times for large relative seperations using the theorems provided in the Appendix B for quenches within one of the phases. For quenches across the critical point, it is possible to consider the behaviour for large relative seperations by using another theorem. These calculations have been performed in [Calabrese et al., 2012b], to which we refer for the derivations. Here, we simply state the results obtained in the aforementioned work. We will use $g = 1$ from now on.

For fixed but asymptotially large relative seperations, r, the quenched correlation function in the thermodynamic limit and for asymptotically large values of the time passed after the sudden quench, t, is given by

$$\bar{C}_r(t \gg g^{-1}, h_1, h_0) \approx E(r, h_1, h_0) e^{-r/\xi(h_1,h_0)} , \tag{4.76}$$

where ξ is the correlation length. For the inverse correlation length, it is possible to give the general formula

$$\begin{aligned} \xi^{-1}(h_1, h_0) = -\frac{1}{2\pi} \int_{-\pi}^{\pi} \log |1 - 2n(k, h_1, h_0)| \, \mathrm{d}k \\ + \Theta(h_1 - 1)\Theta(h_0 - 1) \log \min\{h_0, \bar{h}(h_1, h_0)\} , \end{aligned} \tag{4.77}$$

where $n(k, h_1, h_0)$ denotes the average occupation numbers of the Bogoliubov fermions after a sudden quench from h_0 to h_1, that is,

$$n(k, h_1, h_0) = \left\langle \Omega(h_0) \middle| c_k^\dagger(h_1) c_k(h_1) \Omega(h_0) \right\rangle , \tag{4.78}$$

$\bar{h}$ is a function of the initial and final fields, which is given by

$$\bar{h}(h_1, h_0) = \frac{1 + h_1 h_0 + \sqrt{(h_1^2 - 1)(h_0^2 - 1)}}{h_1 + h_0} , \tag{4.79}$$

and Θ is the Heaviside step function. Depending on the type of the quenches, explicit formulas have been derived for the correlation length ξ and the function E.

1. For sudden quenches within the ferromagnetic phase, $h_0 < 1$ and $h_1 < 1$, we have that

$$E(r, h_1, h_0) = \frac{1 - h_1 h_0 + \sqrt{(1 - h_1^2)(1 - h_0^2)}}{2\sqrt{1 - h_1 h_0}\sqrt{1 - h_0^2}} , \tag{4.80}$$

   and for the inverse correlation length, we have that

$$\xi^{-1}(h_1, h_0) = -\log\left(\frac{h_1 + h_0}{2} \bar{h}(h_1, h_0)\right) . \tag{4.81}$$

2. For sudden quenches within the paramagnetic phase, $h_0 > 1$ and $h_1 > 1$, we have that

$$E(r, h_1, h_0) = \begin{cases} -\dfrac{h_0\sqrt{h_1}(h_1h_0 - 1 + \sqrt{(h_1^2-1)(h_0^2-1)})^2}{4\sqrt{\pi}(h_0^2-1)^{3/4}(h_0h_1-1)^{3/2}(h_1-h_0)} r^{-3/2} & \text{if } 1 < h_0 < h_1, \\ \sqrt{\dfrac{h_1(h_0-h_1)\sqrt{h_0^2-1}}{(h_1+h_0)(h_1h_0-1)}} & \text{if } 1 < h_1 < h_0, \end{cases} \tag{4.82}$$

and for the inverse correlation length, we have that

$$\xi^{-1}(h_1, h_0) = -\log\left(\frac{h_1+h_0}{2h_0h_1}\bar{h}(h_1, h_0)\right) + \log\min\{h_0, \bar{h}(h_1, h_0)\}\,. \tag{4.83}$$

3. For sudden quenches from the the paramagnetic phase to the ferromagnetic phase, $h_0 > 1$ and $h_1 < 1$, we have that

$$E(r, h_1, h_0) = \sqrt{\frac{h_0 - h_1}{\sqrt{h_0^2-1}}} \cos\left(r \arctan\frac{\sqrt{(1-h_1^2)(h_0^2-1)}}{1+h_0h_1}\right)\,, \tag{4.84}$$

and for the inverse correlation length, we have that

$$\xi^{-1}(h_1, h_0) = -\log\left(\frac{h_1+h_0}{2h_0}\right)\,. \tag{4.85}$$

4. For sudden quenches from the the ferromagnetic phase to the paramagnetic phase, $h_0 < 1$ and $h_1 > 1$, we have that

$$E(r, h_1, h_0) = \sqrt{\frac{h_1\sqrt{1-h_0^2}}{h_0+h_1}}\,, \tag{4.86}$$

and for the inverse correlation length, we have that

$$\xi^{-1}(h_1, h_0) = -\log\left(\frac{h_1+h_0}{2h_1}\right)\,. \tag{4.87}$$

4.3 The Space-Time Scaling Limit

In [Calabrese et al., 2012a], analytic expressions for the asymptotic behaviour of the quenched ground state correlation function (4.55) in the thermodynamic limit and for quenches within one of the two phases have been derived in a certain limit, which the authors of the work called the space-time scaling limit. In the remainder of this chapter, we will discuss their results and compare them to our numerical calculation.

For a fixed relative separation, r, the time evolution can be divided into different regimes by means of the propagation velocity of the elementary excitations, $v(k, h)$, which is given by

$$v(k,h) = \frac{\mathrm{d}\omega_k(h)}{\mathrm{d}k}\,. \tag{4.88}$$

For the maximal velocity, we have that $v_{\max}(h) = \max\{v(k,h)\,|\,k \in [-\pi,\pi]\} = 2\min\{h,1\}$. The analytic expressions for the quenched ground state correlation function have been provided for intermediate times which are characterized by the condition that $v_{\max}(h_1)t \propto r$. More precisely, the evolution in time has been considered along rays in space-time, which are given by $\kappa r = v_{\max}(h_1)t$, where κ is some constant. The space-time scaling limit is then given by $v_{\max}(h_1)t \to \infty$ and $r \to \infty$ while κ is kept constant.

The analytic results for the quenched ground state correlation function in the thermodynamic limit have been calculated using two different methods. The first method is based on the representation of the quenched ground state correlation function as a determinant as in (4.55). This method has been developped by the authors of [Calabrese et al., 2012a] and it allowed them to consider the asymptotics of the quenched ground state correlator for quenches within the ferromagnetic phase. The second method uses a Lehmann representation for the quenched correlation function. This results is an expansion in powers of the function K, where

$$K(k,h_1,h_0) = \mathrm{i}\frac{v_k(h_1)u_k(h_0) - u_k(h_1)v_k(h_0)}{u_k(h_1)u_k(h_0) - v_k(h_1)v_k(h_0)}\,. \tag{4.89}$$

This function is related to the mode occupations of the final Bogoliubov fermions with respect to the quenched state by

$$n(k,h_1,h_0) = \frac{K^2(k,h_1,h_0)}{1 + K^2(k,h_1,h_0)}\,. \tag{4.90}$$

This second approach is called the form factor approach by the authors and it gives accurate results only for quenches resulting in small mode occupation numbers after the quench. In particular, the authors emphasize that this form factor approach is not expected to give good results for quenches to or from the close vicinity of the quantum critical point. We will consider their results obtained using the form factor approach only for quenches within the paramagnetic phase since, for quenches within the ferromagnetic phase, the first method based on expression (4.55) is more accurate.

In the following, we give the analytic expressions for the quenched ground state correlation function for quenches within the two phases obtained in [Calabrese et al., 2012a].

Quenches within the Ferromagnetic Phase For quenches within the ferromagnetic phase, for which $h_0 < 1$ and $h_1 < 1$, the first method based on the asymptotic evaluation of the expression (4.55) in the space-time scaling limit gives that

$$\bar{C}_r(t, h_1, h_0) \approx E(r, h_1, h_0) \exp\left(r \int_0^\pi \log|1 - 2n(k, h_1, h_0)|\Theta(2tv(k, h_1) - r)\frac{\mathrm{d}k}{\pi}\right) \times \exp\left(2t \int_0^\pi v(k, h_1) \log|1 - 2n(k, h_1, h_0)|\Theta(r - 2tv(k, h_1))\frac{\mathrm{d}k}{\pi}\right), \quad (4.91)$$

where E is given by (4.80). We emphasize, again, that this is an asymptotic expression derived for $v_{\max}(h_1)t \to \infty$ and $r \to \infty$ while $v_{\max}(h_1)t/r$ is kept constant. Note that since $v_{\max}(h_1) = 2\min\{h_1, 1\}$ and since $h_1 < 1$, we have that $v_{\max}(h_1) = 2h_1$. The dependence on the relative separation on the chain is within the first exponential factor. This factor also involves $\Theta(2v(k, h_1)t - r)$. This implies, that for a fixed r and for $2h_1 t = 2v_{\max}(h_1)t < r$, the first exponential equals to one. Correlations at r arrive from $t = r/(2h_1)$ onward. This means that the correlations spread in a light cone like fashion.

Quenches within the Paramagnetic Phase For quenches within the paramagnetic phase, $h_0 > 1$ and $h_1 > 1$, the form factor approach in the space-time scaling limit gives that

$$\bar{C}_r(t, h_1, h_0) \approx E(r, h_1, h_0)e^{-r/\xi(h_1,h_0)} + \left(h_1^2 - 1\right)^{1/4} \sqrt{4h_1} \int_{-\pi}^{\pi} \frac{K(k, h_1, h_0)}{\omega_k(h_1)} \sin(2t\omega_k(h_1) - kr)\frac{\mathrm{d}k}{\pi} \times \exp\left(-2\int_0^\pi K^2(k, h_1, h_0)\left[r + \Theta(r - 2tv(k, h_1))(2tv(k, h_1) - r)\right]\frac{\mathrm{d}k}{\pi}\right), \quad (4.92)$$

where E is given by (4.82). Note that since $v_{\max}(h_1) = 2\min\{h_1, 1\}$ and since $h_1 > 1$, we have $v_{\max}(h_1) = 2$. We again observe a light cone like propagation of the correlations. Based on this result, which is obtained by the form factor approach, the authors conjecture the form of the full correlation function,

$$\bar{C}_r(t, h_1, h_0) \approx \left(E(t, h_1, h_0) + \left(h_1^2 - 1\right)^{1/4} \sqrt{4h_1} \int_{-\pi}^{\pi} \frac{K(k, h_1, h_0)}{\omega_k(h_1)} \sin(2t\omega_k(h_1) - kr)\frac{\mathrm{d}k}{\pi}\right) \times \exp\left(\int_0^\pi \log|1 - 2n(k, h_1, h_0)|\left[r + \Theta(r - 2tv(k, h_1))(2tv(k, h_1) - r)\right]\frac{\mathrm{d}k}{\pi}\right) \quad (4.93)$$

4.4 Sudden Quenches to the Vicinity of the Quantum Critical Point

In the context of this work, we are interested in the correlation function of the order parameter, X_j, with respect to the quenched state. By using the expression (4.55), we are able to numerically evaluate the quenched ground state correlation function for any choice of N and for any values of the initial and final fields h_0 and h_1. Note, that we are still using $g = 1$, which also sets the units of energy and momentum.

In practice, we considered quenches from a large initial field, h_0, effectively corresponding to the limit $h_0 \to \infty$, to the vicinity of the quantum critical point within the paramagnetic phase, that is, $h_1 = 1 + \varepsilon$ for small positive numbers ε. We also use a large value for N in our calculations of the quenched ground state correlation function. Comparisons with calculations performed using the thermodynamic limit show that, for large enough N, their difference is negligible. This is, of course, not surprising since we already realized in Section 4.2 that the thermodynamic limit is simply the limit $N \to \infty$ of (4.55). The reason for why we use calculations with large N instead of the exact expressions for the thermodynamic limit is that the limit involves integrals, which take longer to be evaluated on the computer but do not show significant differences to the large N computation. Even if we would use the expressions in the thermodynamic limit involving integrals, when evaluated numerically, they would be discretized anyway. However, we need to take into account that due to the periodic boundary condition, the local perturbations initially starting at the origin move in opposite directions and meet after a certain time. Therefore, after identifying this time value for fixed and large values of N, we only consider the time evolution for times smaller than this value. Of course, the larger the chain, the larger will be this time span. We find that the value $N = 400$ is high enough since it allows us to consider the evolution in time of the quenched ground state correlation function for sufficiently long times to observe the characteristic behaviour and is compatible with the thermodynamic limit as described above.

We will compare our numerical calculations with the analytical expressions derived in [Calabrese et al., 2012a,b] in the following. We already presented the relevant formulas in the preceding sections, namely Section 4.2 and Section 4.3. For the quenches which we are considering, we need to compare our results to the equations (4.92) and (4.93). Thereby, the first equation is obtained by the form factor approach which is only valid for quenches which result in small mode occupations of the final Bogoliubov fermions after the sudden quench. The second expression is a guess of the authors based on the first equation. Since the validity of (4.92) depends on the mode occupations after the quench, we need to consider them first. In Figure 4.1, we show

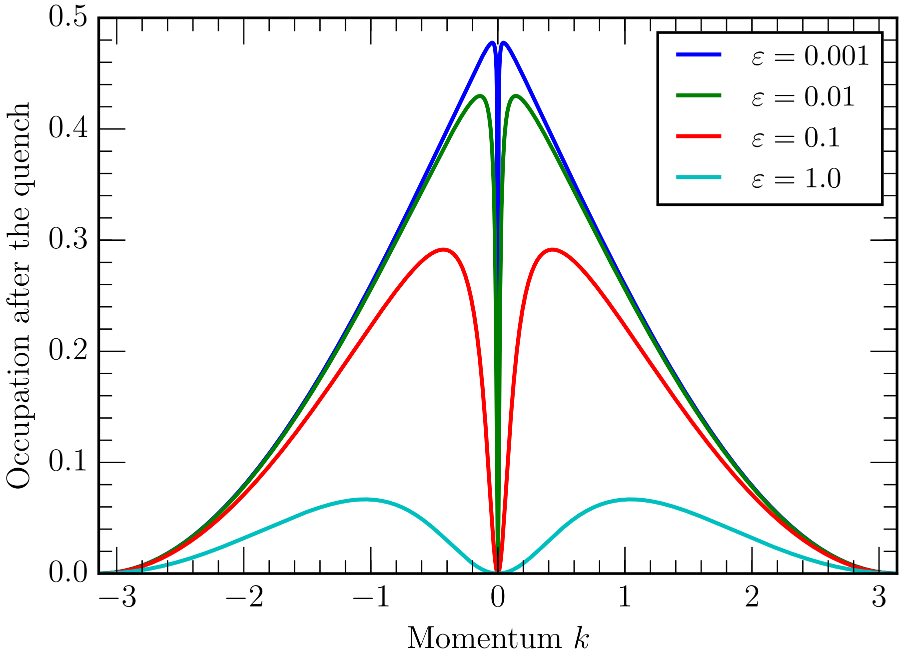

Figure 4.1: Occupation numbers of the Bogoliubov fermions with respect to the quenched state as a function of the momentum p in the interval $[-\pi, \pi]$. The curves are all calculated for an initial field $h_0 = 1000$, but different final fields $h = 1 + \varepsilon$. The closer we get to the quantum critical point, the larger the occupations become.

numerically evaluated post-quench occupation numbers for sudden quenches from $h_0 = 1000$ to the vicinity of the quantum critical point for different values of ε. We find that the closer we get to the quantum critical point, the larger the occupation numbers become. This renders the expression (4.92) invalid close to the quantum critical point. This can be observed directly in the Figures 4.2 and 4.3, where we have plotted (4.92) (green curve) and our numerical data (red curve) for six different times and for $\varepsilon = 0.1$ and $\varepsilon = 0.001$, respectively.

In Equation (4.93), the authors of [Calabrese et al., 2012a] conjecture the generic form of the correlation based on expression (4.92). We used the formula to compare it with our numerical calculations. The comparison is given in the Figures 4.2 and 4.3, where we have plotted this expression (magenta curve) and our numerical data (red curve) for $\varepsilon = 0.1$ and $\varepsilon = 0.001$, respectively. We observe very good agreement close to the quantum critical point. However, the further away we go from the quantum critical point, the worse becomes the agreement. This is not surprising since, for

$h_0 \to \infty$, the inverse correlation length ξ^{-1}, given in (4.77), reduces to

$$\lim_{h_0\to\infty} \xi^{-1}(h_1, h_0) = -\lim_{h_0\to\infty} \int_0^{\pi} \log|1 - 2n(k, h_1, h_0)| \frac{\mathrm{d}k}{\pi} + \ln(h_1 + \sqrt{h_1^2 - 1})\,. \quad (4.94)$$

Therefore, the first summand in (4.92) differs from the first summand of (4.93), since the correlation length, for large values of t, differs by the term $\ln(h_1 + \sqrt{h_1^2 - 1})$, as can be seen in (4.94). This additional term decreases as h_1 tends to the quantum critical point from above, eventually vanishing for $h_1 = 1$. In this limit, the two expressions match.

So far, we observed that the formulas (4.92) and (4.93) describe two different regimes. The first formula agrees with our numerical calculations for quenches further away from the quantum critical point, where the mode occupations of the final Bogoliubov fermions after the quench are small. The second expression describes the numerical calculations well for quenches close to the quantum critical point. Based on these two formulas, we propose a new formula to remedy the deficiencies. Our conjecture reads

$$\begin{aligned}\bar{C}_r(t, h_1, h_0) \approx\ & E(r, h_1, h_0) e^{-r/\xi(h_1,h_0)} \\ & + \left(h_1^2 - 1\right)^{1/4} \sqrt{4h_1} \int_{-\pi}^{\pi} \frac{K(k, h_1, h_0)}{\omega_k(h_1)} \sin(2t\omega_k(h_1) - kr) \frac{\mathrm{d}k}{\pi} \\ & \times \exp\left(\int_0^{\pi} \log|1 - 2n(k, h_1, h_0)| \left[r + \Theta(r - 2tv(k, h_1))(2tv(k, h_1) - r)\right] \frac{\mathrm{d}k}{\pi} \right)\,, \end{aligned} \quad (4.95)$$

where E is given by (4.82), and does not depend on r, and ξ^{-1} is given by (4.83). This guess is motivated by the following considerations: The second exponential in our formula involves the lograrithm $\log|1-2n(k, h_1, h_0)|$. The expression $1-2n(k, h_1, h_0)$ is positive for the quenches which we consider. Thus, we do not need to take the absolute value. Further, we have that

$$1 - 2n(k, h_1, h_0) = \frac{1 - K^2(k, h_1, h_0)}{1 + K^2(k, h_1, h_0)}\,,$$

where the function K is given in (4.89). We can expand the logarithm to obtain

$$\log|1 - 2n(k, h_1, h_0)| = -\sum_{n=1}^{\infty} \frac{1}{n}(1 - (-1)^n) K^{2n}(k, h_1, h_0)\,.$$

In particular, the first term in the expansion is $-2K^2(k, h_1, h_0)$. Thus, expression (4.92) agrees with the leading term of the expansion in K of our formula.

Formula (4.95) encompasses the advantages of both of the Equations (4.92) and (4.93), and agrees reasonably well with our numerical calculations for a wide range of values of ε. This can be seen, again, in the Figures 4.2 and 4.3, where we have depicted (4.95) in blue. Therefore, for our further considerations, we will use the improved formula (4.95).

Although the formulas (4.92), (4.93), and (4.95) (since it is based on the first two expressions) should be only valid for sufficiently large values of r and t, we observe in the Figures 4.2 and 4.3 that they describe the correlations within the cone of propagation right from the outset. In particular, our formula suggests that there is a crossover scale on the lattice. Below this scale, the correlation function is dominated by the first summand in (4.95), which is nothing else but the stationary value for the quenched ground state correlation function given by a generalized Gibbs ensemble. From this scale onward, the second summand in the same formula dominates the form of the correlation function. This can be seen clearly in Figure 4.4. In Figure 4.2, we can observe that this crossover scale changes slowly as a function of the time passed after the sudden quench. In Figure 4.4, we can also see that for long times after the quench, we are able to identify two correlation lengths ξ_1 and ξ_2. The first one is given by the generalized Gibbs ensemble, that is, $\xi_1(h_1, h_0) = \xi(h_1, h_0)$. Explicitly, we have that

$$\xi_1^{-1}(h_1, h_0) = -\frac{1}{2\pi}\int_{-\pi}^{\pi} \log|1 - 2n(k, h_1, h_0)|\,\mathrm{d}k + \log\min\{h_0, \bar{h}(h_1, h_0)\}\,, \quad (4.96)$$

where $\bar{h}$ is given in (4.79). The inverse of the second correlation length is given by

$$\xi_2^{-1}(h_1, h_0) = -\frac{1}{2\pi}\int_{-\pi}^{\pi} \log|1 - 2n(k, h_1, h_0)|\,\mathrm{d}k\,. \quad (4.97)$$

The inverses of the two correlation lengths differ by $\log\min\{h_0, \bar{h}(h_1, h_0)\}$, which vanishes for $h_1 = 1$. Therefore, for quenches to the critical point, there is only one correlation length characterizing the quenched ground state correlation function and, thus, there is also no crossover. If we consider quenches from $h_0 \to \infty$ to h_1, then the difference of the inverse correlation lengths is given by $\lim_{h_0\to\infty} \bar{h}(h_1, h_0) = h_1 + \sqrt{h_1^2 - 1}$. This decreases as h_1 comes closer to the quantum critical point within the paramagnetic phase. Therefore, we can characterize the correlation function by one correlation length already for small distances ε from the quantum critical point. This can be seen in Figure 4.3. That is, close to the quantum critical point, the correlation length is the one obtained from the generalized Gibbs ensemble.

In any case, we observe that at short distances on the lattice, the quenched ground state correlation function is characterized by the generalized Gibbs ensemble. To further strengthen this claim, we fitted an exponential decay to the values of the quenched ground state correlation function on the first ten points of the lattice and compared the therewith obtained correlation length to the one given by the

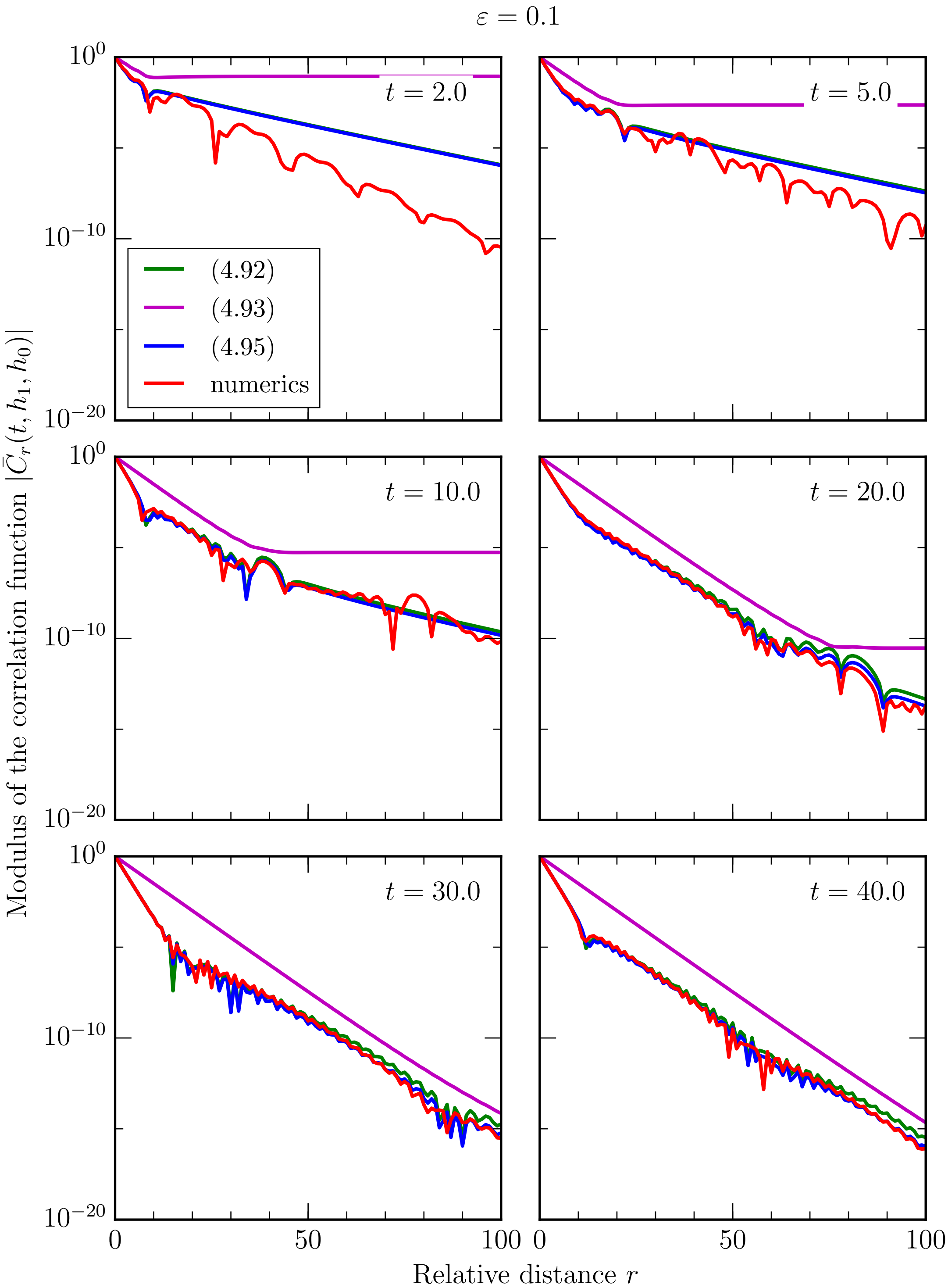

Figure 4.2: Comparison of the numerically evaluated correlator with the equations (4.92), (4.93), and (4.95). The numerical data is given by the red curve. Equation (4.92) is green, equation (4.93) is magenta, and equation (4.95) is blue. The curves are depicted for four different values of t and for $\varepsilon = 0.1$.

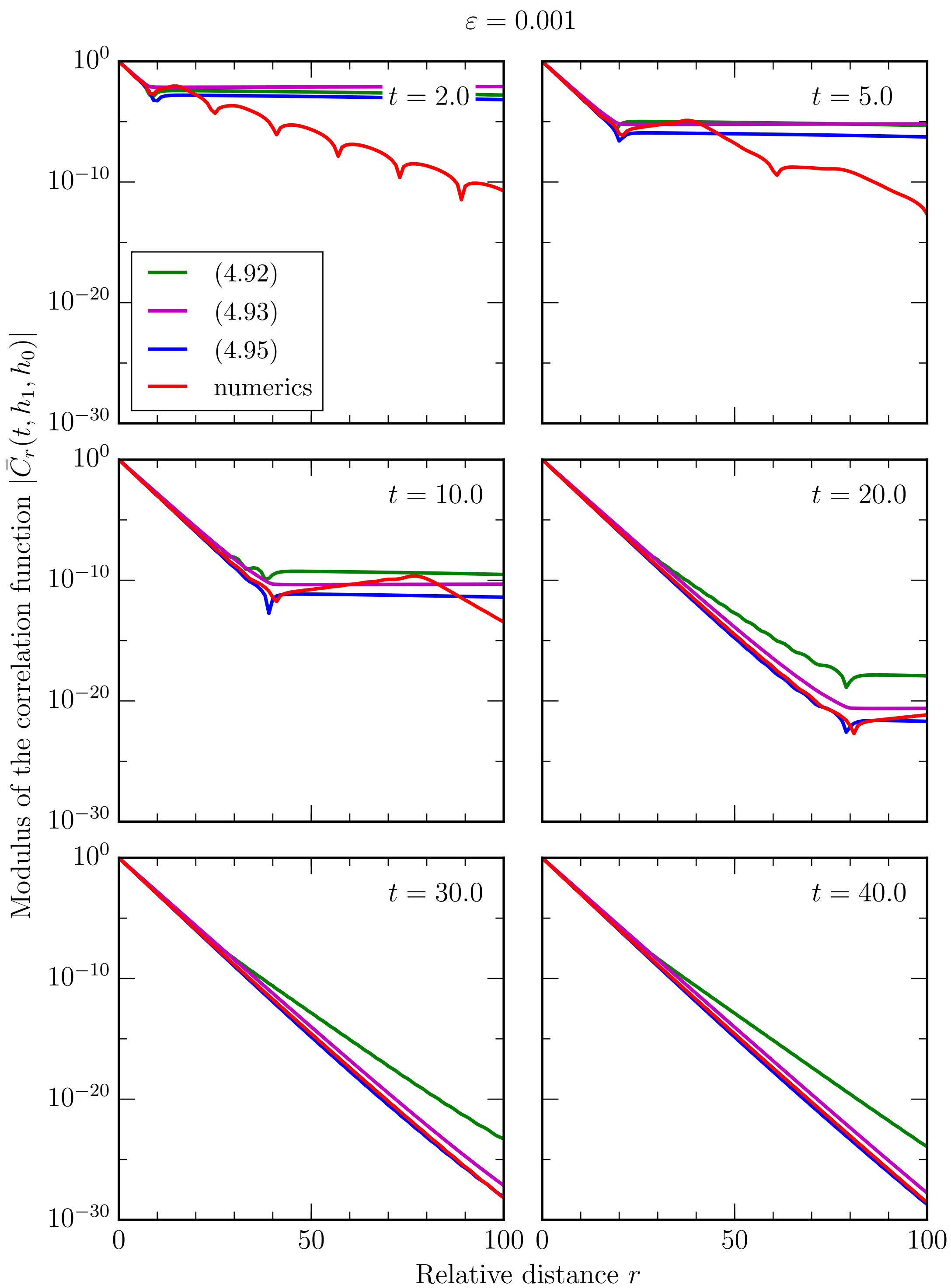

Figure 4.3: Comparison of the numerically evaluated correlator with the equations (4.92), (4.93), and (4.95). The numerical data is given by the red curve. Equation (4.92) is green, equation (4.93) is magenta, and equation (4.95) is blue. The curves are depicted for four different values of t and for $\varepsilon = 0.001$.

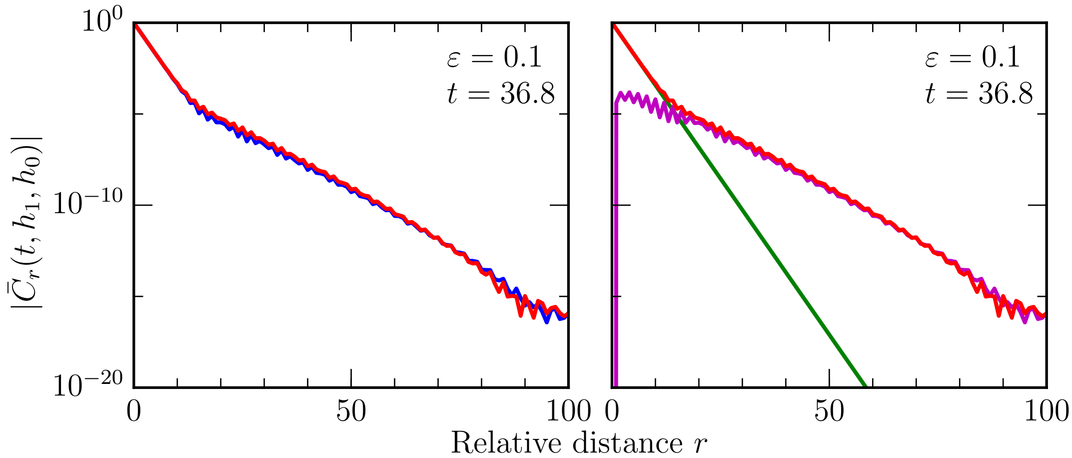

Figure 4.4: The correlation function for $h_0 = 1000$ and $\varepsilon = 0.1$ at time $t = 36.8$. (Left plot) The red curve represents the numerical data, while the blue curve is given by equation (4.95). (Right plot) The red curve represents again the numerical calculation. The green curve is the first summand of (4.95) and the magenta curve is the second summand. Up to some length scale (here, approximately given by 15 sites), the correlator is given by the first summand of (4.95). From this length scale onward, the second term of the same formula dominates the correlator.

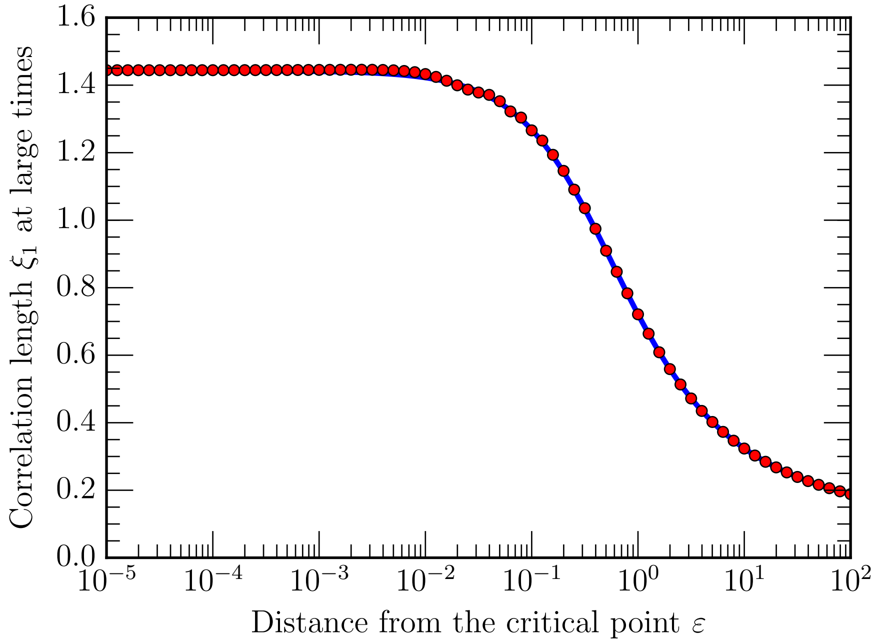

Figure 4.5: The correlation length obtained from the fit to the first ten points of our numerical calculations for a fixed time. The time value is chosen such that the decay over the first ten points is observable in the numerics. The red points are the results of the fit and the blue curve is the correlation length obtained from the generalized Gibbs ensemble. We used the generalized Gibbs ensemble result for the correlation length in the limit $h_0 \to \infty$, which is given by $1/\log(2h_1)$.

generalized Gibbs ensemble, ξ_1, for different values of h_1. We depicted the result in the Figure 4.5. We can clearly see an agreement with the correlation length given by the generalized Gibbs ensemble.

In summary, we demonstrated that the short-distance decay of the order parameter correlation function after the sudden quench is described by the correlation length obtained by the generalized Gibbs ensemble right after the quench. This is interesting because one would expect to see the stationary values only for asymptotically large times after the quench.

The correlation lengths are mainly determined by the occupation numbers of the final Bogoliubov fermions after the sudden quench. For this reason, we want to understand them in more detail.

We shortly summarize what we already know about these occupation numbers. In Section 4.2, we related the final Bogoliubov operators, $c_p(h_1)$, to the initial Bogoliubov operators, $c_p(h_0)$, by the relation $c_p(h_1) = f_p(h_1, h_0)c_p(h_0) + g_p(h_1, h_0)c^\dagger_{-p}(h_0)$, where the expressions $f_p(h_1, h_0)$ and $g_p(h_1, h_0)$ are given in (4.73) and (4.74). The occupation numbers of the final Bogoliubov fermions after the sudden quench are then given by $n(p, h_1, h_0) = |g_p(h_1, h_0)|^2$. More explicitly, for all $p \in \mathbb{R}$ with $p \notin \pi\mathbb{Z}$, we have that

$$n(p, h_1, h_0) = \frac{1}{2} - \frac{1}{2} \frac{h_0 h_1 - g(h_0 + h_1)\cos p + g^2}{\sqrt{g^2 + h_0^2 - 2gh_0 \cos p}\sqrt{g^2 + h_1^2 - 2gh_1 \cos p}}\,, \tag{4.98}$$

and for all $p \in \pi\mathbb{Z}$, we find that

$$n(p, h_1, h_0) = 0\,. \tag{4.99}$$

The occupation numbers are 2π-periodic, and, thus, we restrict our attention to the intervall $[-\pi, \pi]$.

The first question we are going to consider is, why these occupation numbers are zero at zero momentum, as can be seen in Figure 4.1. The relation between the final Bogoliubov fermions and the initial one is given by a Bogoliubov transformation with the factors being $f_p(h_1, h_0)$ and $g_p(h_1, h_0)$. Therefore, we can relate the vacuum state of the operators $c_p(h_1)$, which is represented by $\tilde{\Omega}(h_1)$, to the vacuum state of the operators $c_p(h_0)$, which is represented by $\tilde{\Omega}(h_0)$, where $p \in P_N$. Thereby, the rationale is the same as in Section 2.5, where we related the Bogoliubov vacuum to the Jordan-Wigner vacuum. Namely, we obtain that

$$\tilde{\Omega}(h_0) \propto \exp\left(-\sum_{p \in P_N^+} \frac{g_p^*(h_1, h_0)}{f_p^*(h_1, h_0)} c_p^\dagger(h_1) c_{-p}^\dagger(h_1)\right) \tilde{\Omega}(h_1)\,, \tag{4.100}$$

where we left the normalization factor unspecified. With the help of this identity, we can see that the vacuum of the initial Bogoliubov operator, $c_p(h_0)$, contains only pairwise excitations of the vacuum of the final Bogoliubov operators, $c_p(h_1)$, with positive and corresponding negative momenta. In particular the $p = 0$ and the $p = \pm\pi$ modes are not excited. Thus, the mode occupation number of the final Bogoliubov fermions after the quench are zero for these values of the momentum.

The second question we are asking is, whether the mode occupation numbers of the final Bogoliubov fermions after the quench can be described by a thermal distribution with an appropriately defined temperature. That is, can the occupation numbers be described by a Fermi-Dirac distribution? The answer to this question is that, for quenches from $h_0 \to \infty$ to $h_1 = 1$, we can use a thermal description to a certain extend. Namely, for all $p \in \mathbb{R}$ with $p \notin \pi\mathbb{Z}$, we have that

$$n(p, h_1 = 1, h_0 \to \infty) = \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\sqrt{1 - \cos p}\right)\,. \tag{4.101}$$

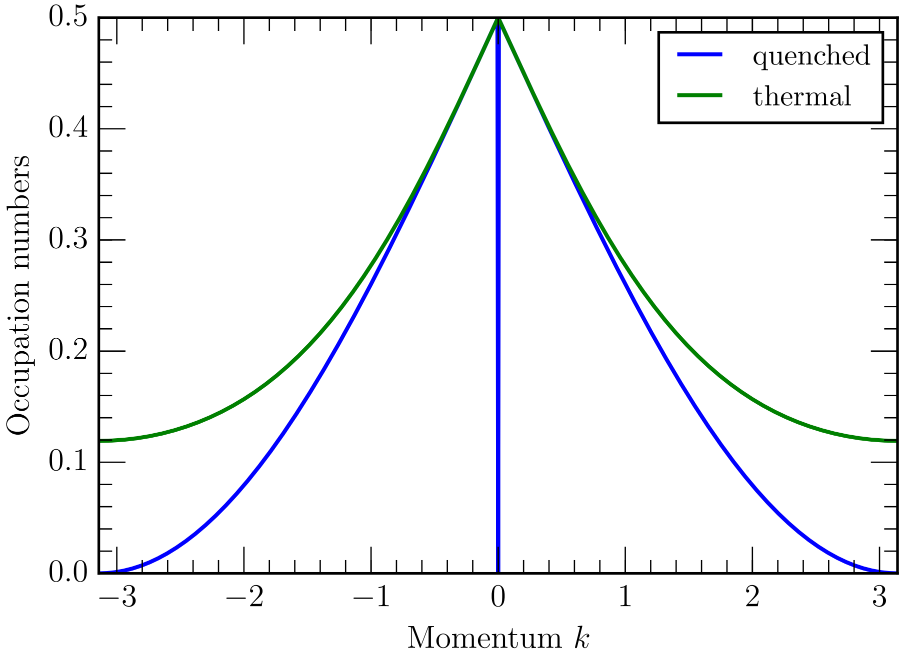

Figure 4.6: The occupation numbers of the final Bogoliubov fermions after the sudden quench from $h_0 \to \infty$ to $h_1 = 1$ compared to the thermal distribution of the final Bogoliubov fermions with an effective temperature 2. The occupations after the quench are given by the blue curve and the thermal distribution is depicted blue. We observe that these two results are approximately the same for momenta for which the dispersion is small, as can be seen in Figure 2.1.

For the Fermi-Dirac distribution with inverse temperature β, we obtain that

$$\begin{aligned}\left(e^{-\beta\omega_p(h_1=1)}+1\right)^{-1} &= \left(1+1+2\beta\sqrt{2(1-\cos p)}+\mathcal{O}(\beta^2\omega_p^2(h_1=1))\right)^{-1} \\ &= \frac{1}{2}\left(1+\beta\sqrt{2(1-\cos p)}+\mathcal{O}((\beta\omega_p(h_1=1)/2)^2)\right)^{-1} .\end{aligned}$$

If we now assume that $\beta^2\omega_p^2(h_1=1) \ll 1$, then we have that

$$\left(e^{-\beta\omega_p(h_1=1)}+1\right)^{-1} \approx \frac{1}{2}\frac{1}{1+\beta\sqrt{2(1-\cos p)}} \approx \frac{1}{2}\left(1-\beta\sqrt{2}\sqrt{1-\cos p}\right) .$$

If we now take the effective temperature to be $T = 2$, that is, $\beta = 1/2$, then this expression would agree with (4.101). However, we observe that $\omega_p(h_1 = 1) = 2\sqrt{2(1-\cos p)}$ and thus $\beta\omega_p(h_1 = 1)/2 = \sqrt{(1-\cos p)/2}$, which can be of order one. The expansion is only valid for p such that $\omega_p(h_1 = 1)$ is small. This can be also seen in Figure 4.6.

5 Summary and Conclusions

In this thesis, we considered the dynamics of the Ising chain in a transverse field after a sudden quench. We reviewed the diagonalization of the Hamiltonian in detail and saw that the eigenvalues and eigenstates can be determined by first expressing the Hamiltonian in terms of fermionic Jordan-Wigner operators, followed by a Fourier and Bogoliubov transformation. In terms of the Bogoliubov fermions, the Hamiltonian takes the form of a non-interacting fermionic system in certain subspaces of the Hilbert space of the transverse Ising chain. We also analyzed the structure of the ground state and found that, in the thermodynamic limit, the system has a quantum critical point which separates the ferromagnetic from the paramagnetic phase. We determined the ground state spin correlations and found that the formalism used to determine them applies also for the calculation of spin correlations after a sudden quench if the corresponding functions are defined in an appropriate way. We obtained an expression for the quenched correlator in terms of a Pfaffian, which we then reduced to the determinant of a Toeplitz plus Hankel matrix using only matrix transformations and basic properties of the Pfaffian and determinant. With this, we have put forward a reduction scheme which is simpler and more comprehensive than the corresponding one in [Calabrese et al., 2012a]. Furthermore, this reduction to a determinant allowed us to calculate the spin correlations after a sudden quench in an efficient way.

In [Calabrese et al., 2012b], it is argued that the transverse Ising chain approaches asymptotically a stationary state given by an generalized Gibbs ensemble which accounts for the occupation operators of the Bogoliubov fermions. We reconstructed this argument by considering the long time asymptotics of the longitudinal correlation function in the thermodynamic limit after a sudden quench. Then, we turned our attention to sudden quenches from initially large fields to the vicinity of the quantum critical point within the paramagnetic phase. For such quenches, we improved expressions from [Calabrese et al., 2012a] describing the large time and distance asymptotics of the quenched longitudinal correlator. Our improved formula is given by Equation (4.95). Our numerical calculations as well as this conjectured formula showed that there are two correlation lengths characterizing the decay of the longitudinal correlation function, one of which is the correlation length obtained from the generalized Gibbs ensemble. In particular, the quenched longitudinal correlation function attains its stationary values already at short distances and these values are characterized by the generalized Gibbs ensemble. This is an unexpected observation since the generalized Gibbs ensemble expressions have been derived for large relative seperations. This result is especially important for experiments since it implies that stationarity can be observed on short distances and times. That the transverse field Ising chain is not only of theoretical interest was shown in [Nicklas et al., 2015]. There, quenches to the close vicinity of the critical point in a two-component Bose gas have been experimentally realized and they succeded in observing scaling in the dynamics. Moreover, numerical calculations showed that the dependence of the correlation length on the distance from the critical point is reminiscent of the universal crossover behaviour of an equilibrium one-dimensional Ising system.

Since the correlation lengths characterizing the decay of the longitudinal spin correlator after the sudden quench are related to the occupations of the Bogoliubov fermions after the sudden quench, we examined these occupations in more detail. We found that these mode occupations can be described by a thermal distribution with an effective temperature of two in units of the spin interaction coupling energy for a certain range of modes where the dispersion of the Bogoliubov fermions is small enough.

The Ising chain in a transverse field attracted a lot of attention in the context of quench dynamics since it is integrable and the calculations are amenable. There are a lot of works concerned about quenches in this model but we find the most developed analysis is provided in [Calabrese et al., 2012a,b]. However, although the calculations in these two works have been performed for the transverse Ising chain, we think that it should be straightforward to translate these results to more general spin models like the XY chain.

A Jordan-Wigner Operators

Here, we prove that the Jordan-Wigner operators given by (2.7) satisfy the canonical anticommutation relations

$$a_j a_k + a_k a_j = 0\,, \tag{A.1}$$

$$a_j a_k^\dagger + a_k^\dagger a_j = \delta_{jk}\,. \tag{A.2}$$

Let $[\cdot,\cdot]$ denote the commutator and let $\{\cdot,\cdot\}$ denote the anticommutator. For σ_j defined in (2.5), we have that $\{\sigma_j,\sigma_j\} = 0$ and that $\left\{\sigma_j,\sigma_j^\dagger\right\} = 1$. From these relations, it follows that the operators $\sigma_j^\dagger\sigma_j$ are idempotent. This, in turn, implies that

$$\exp\left(\mathrm{i}\pi\sigma_j^\dagger\sigma_j\right) = I - 2\sigma_j^\dagger\sigma_j = Z_j\,.$$

Therefore, by using (2.7), we can rewrite the Jordan-Wigner operators as

$$a_j = \left[\prod_{k=0}^{j-1} Z_k\right]\sigma_j\,. \tag{A.3}$$

We will use this form in the following to prove the canonical anticommutation relations.

Let us first prove the identity (A.1). Let $j < k$. Then, we have that

$$\begin{aligned}\{a_j,a_k\} &= \left[\prod_{l=0}^{j-1} Z_l\right]\sigma_j\left[\prod_{m=0}^{k-1} Z_m\right]\sigma_k + \left[\prod_{m=0}^{k-1} Z_m\right]\sigma_k\left[\prod_{l=0}^{j-1} Z_l\right]\sigma_j \\ &= \left[\prod_{l=j}^{k-1} Z_l\right]\left(Z_j\sigma_j Z_j\sigma_k + \sigma_k\sigma_j\right)\,.\end{aligned}$$

We have that $[Z_j,\sigma_j] = \frac{1}{2}[Z_j,X_j] + \frac{\mathrm{i}}{2}[Z_j,Y_j] = 2\sigma_j$. This identity implies that $[Z_j,[Z_j,\sigma_j]] = 4\sigma_j$. On the other hand, writing out $[Z_j,[Z_j,\sigma_j]]$ results in the identity $[Z_j,[Z_j,\sigma_j]] = 2\sigma_j - 2Z_j\sigma_j Z_j$. Therefore, we obtain that $Z_j\sigma_j Z_j = -\sigma_j$. This gives

$$\{a_j,a_k\} = \left[\prod_{l=j}^{k-1} Z_l\right]\left(\sigma_k\sigma_j - \sigma_j\sigma_k\right) = 0\,.$$

For $j = k$, we have that

$$\{a_j,a_k\} = 2a_j^2 = 2\sigma_j^2 = \frac{\mathrm{i}}{2}\{X_j,Y_j\} = 0\,.$$

For $j > k$, we can interchange the labels j and k and use the symmetry of the anticommutator to reduce this case to the first one. Thus, we have proven that $\{a_j, a_k\} = 0$ for any j and k.

Now, let us prove the identity (A.2). Let $j < k$. Then, we have that

$$\begin{aligned}\left\{a_j, a_k^\dagger\right\} &= \left[\prod_{l=0}^{j-1} Z_l\right] \sigma_j \left[\prod_{m=0}^{k-1} Z_m\right] \sigma_k^\dagger + \left[\prod_{m=0}^{k-1} Z_m\right] \sigma_k^\dagger \left[\prod_{l=0}^{j-1} Z_l\right] \sigma_j \\ &= \left[\prod_{l=j}^{k-1} Z_l\right] \left(Z_j \sigma_j Z_j \sigma_k^\dagger + \sigma_k^\dagger \sigma_j\right) \\ &= \left[\prod_{l=j}^{k-1} Z_l\right] \left(\sigma_k^\dagger \sigma_j - \sigma_j \sigma_k^\dagger\right) \\ &= 0\,.\end{aligned}$$

For $j = k$, we have that

$$\left\{a_j, a_j^\dagger\right\} = \left\{\sigma_j, \sigma_j^\dagger\right\} = 1\,.$$

For $j > k$, we can use that $\left\{a_j, a_k^\dagger\right\} = \left\{a_k, a_j^\dagger\right\}^\dagger$ and interchange the labels j and k to reduce this case to the first one. Thus, we have proven that $\left\{a_j, a_k^\dagger\right\} = \delta_{jk}$ for any j and k.

B Asymptotics of Toeplitz Determinants

We present two results on the asymptotic values of determinants of Toeplitz matrices obtained by Albrecht Böttcher and Harold Widom in [Böttcher and Widom, 2006]. The following statements are taken from the aforementioned work, to which we refer for the proofs.

Let $S^1 \coloneqq \{z \in \mathbb{C} \,|\, |z| = 1\}$ be the complex unit circle and let $f : S^1 \longrightarrow \mathbb{C}$ be an integrable function. The Fourier coefficients, f_k, $k \in \mathbb{Z}$, of f are given by

$$f_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(e^{\mathrm{i}p}) e^{-\mathrm{i}pk} \, \mathrm{d}p \,. \tag{B.1}$$

For any positive integer n, let $T_n(f)$ denote the n by n Toeplitz matrix generated by f, that is, $T_n(f) \coloneqq (f_{j-k})_{j,k=1}^{n}$. Let also $D_n(f) \coloneqq \det T_n(f)$.

Assume that $f : S^1 \longrightarrow \mathbb{C}$ is a function which is continuous and nowhere zero on the complex unit circle S^1. Let $\gamma \in \mathbb{Z}$ denote its winding number about the origin. We can write $f(z) = z^\gamma a(z)$ for any $z \in S^1$, where a is a continuous function on S^1 which has no zeros on S^1 and which has a vanishing winding number about the origin. We assume that a (or, equivalently, f) belongs to C^β for some $\beta > 1/2$ and $\beta \notin \mathbb{N}$. This means that a has $\lfloor \beta \rfloor$ continuous derivatives and the $\lfloor \beta \rfloor$th derivative satisfies a Hölder condition with exponent $\beta - \lfloor \beta \rfloor$. Under these assumptions, the logarithm of a, $\log a$, is in C^β. We denote its Fourier coefficients by $(\log a)_k$ for $k \in \mathbb{Z}$.

Let $G(a) \coloneqq \exp(\log a)_0$. Futhermore, define the functions a_- and a_+ on S^1 by

$$a_-(z) \coloneqq \exp \sum_{k=1}^{\infty} (\log a)_{-k} z^{-k} \,, \tag{B.2}$$

$$a_+(z) \coloneqq \exp \sum_{k=1}^{\infty} (\log a)_{+k} z^{+k} \tag{B.3}$$

for any $z \in S^1$. Since a belongs to C^β, $a_-^{\pm 1}$ and $a_+^{\pm 1}$ belong to C^β as well. We also define the expression

$$E(a) \coloneqq \exp \sum_{k=1}^{\infty} k (\log a)_{-k} (\log a)_k \,. \tag{B.4}$$

Theorem B.1 (Szegö's strong limit theorem)**.** Under the above assumptions on a, we have

$$D_n(a) = G(a)^n E(a) (1 + \mathcal{O}(n^{1-2\beta})) \,. \tag{B.5}$$

Theorem B.2 (Fisher, Hartwig, Silbermann et al.)**.** For a positive integer κ and for any $z \in S^1$, let $g(z) \coloneqq z^{-\kappa} a(z)$ and let $h(z) \coloneqq z^{-n} a_-(z)/a_+(z)$. Then, under the above assumption on a, we have

$$D_n(g) = (-1)^{n\kappa} G(a)^{n+\kappa} E(a)(\det T_\kappa(h) + \mathcal{O}(n^{-3\beta}))(1 + \mathcal{O}(n^{1-2\beta}))\,. \tag{B.6}$$

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Erklärung:

Ich versichere, dass ich diese Arbeit selbstständig verfasst habe und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe.

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