

Exact Short-Distance Correlations of the Heisenberg Chain by Means of the Fermionic Basis

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Chapter 1

Introduction

In this work our goal will be to study static two-point correlation functions of the Heisenberg chain for small distances. The Heisenberg chain, which is also called the XXZ chain, is described by the Hamiltonian

$$H_{XXZ} = J \sum_{k=-\infty}^{\infty} (\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta (\sigma_k^z \sigma_{k+1}^z - 1)) - \frac{h}{2} \sum_{k=-\infty}^{\infty} \sigma_k^z ,$$
$$\Delta = \frac{1}{2}(q + q^{-1}) . \quad (1.1)$$

The σ_k^α are Pauli matrices which act on lattice site k , Δ is the anisotropy parameter, J the strength of the exchange coupling and h an external field in z -direction. The Heisenberg model describes a magnetic insulator and is the fundamental model for the description of antiferromagnetism in solids [1]. The one-dimensional Heisenberg model is of particular interest to us because it is integrable. Integrable models are of interest, since exact solvability is a very rare property for many-particle systems. An overview of the applications of the Heisenberg model as well as the related Hubbard model in solid state physics can be found in [2, 3]. The model was first studied by Bethe in 1931 [4] for $\Delta = 1$ and later for general Δ in [5–8]. The particular case of $\Delta = 1$ is also called the XXX model. Later it was discovered that the Heisenberg model is linked to the so-called six-vertex model of statistical physics [9–12] which added to our understanding of the model. After that the original method of Bethe was further developed to the so-called algebraic Bethe ansatz [13, 14]. In [15–18] the technique of the quantum-transfer matrix was introduced, which can be used to calculate the thermodynamic properties of the XXZ model [18].

To motivate our interest in the study of short-distance static correlation functions it should be noted that they can be observed experimentally using various techniques. The experiments which are most relevant for our work are electron spin resonance (ESR) measurements. Using linear response theory, the moments of absorption lines can be related to short-distance static

correlations [19–22]. An example for this is [23–25] where the authors used the compound $\text{Cu(py)}_2\text{Br}_2$ in ESR experiments and found a good agreement with the next-nearest neighbour functions obtained by theory.

Another example where correlation functions can be observed are neutron scattering experiments [26, 27] that measure the dynamic structure factor of the Heisenberg chain, which is connected to the dynamic two-point correlations. In [28–30] the two- and four-spinon contributions to the dynamic structure factor were calculated. Another measurable physical quantity is the thermal conductivity of the chain which is determined by the dynamic current-current correlation and thus by six-point dynamic correlation functions [31]. Such functions cannot be calculated as of today. The Drude weight however, i.e. the zero frequency component of the thermal conductivity can be studied using various other techniques [31–34]. The predicted behaviour could then be verified in experimental works [35–37]. Even though the neutron scattering and especially the heat transport examples are not directly connected to our goal of calculating short-distance static correlation functions, they make it obvious that studying correlations of the Heisenberg chain is a worthwhile goal.

Apart from experiments there is of course a motivation to study the Heisenberg model from the viewpoint of theoretical physics as well. Interacting many-particle systems cannot ordinarily be solved exactly. As such, two techniques which are used frequently in many-particle physics are perturbation theory and simulations using large computer clusters. Both methods obviously are restricted regarding the generality of their results. Integrable systems like the Heisenberg chain present a different possibility to study many-particle systems since many of their properties can be calculated exactly. Even though integrability is a strong restriction too, the study of integrable systems may contribute to our understanding of more generic many-particle systems. Even a better understanding of the differences between integrable and non-integrable models may help in advancing the generic theory. Additionally, a better understanding of the integrable structure of the Heisenberg chain may help our understanding of integrable systems in other fields like e.g. conformal field theory [38–40]. At last, in our opinion a better understanding of the structure of correlations of the Heisenberg model is a worthwhile goal on its own.

In recent years there has been significant progress in understanding the correlation functions of local operators of integrable spin- $\frac{1}{2}$ chains. The development started when Jimbo et al. [41–43] found explicit expressions for the density matrix of a finite subchain of the infinite XXZ chain at zero temperature and with a vanishing magnetic field. Here the density matrix was expressed in terms of multiple integrals. This was later extended to a non-vanishing magnetic field in [44] and to finite temperatures in [45].

The next big step was the discovery that these multiple integrals can be factorized [46] and that the resulting integrals can be written in an exponential

form [47, 48]. This made it possible to distinguish between an algebraic part and a physical part. The algebraic part is tied to the representation theory of the model's symmetry algebra. In our case this will be the XXZ chain, so the corresponding quantum group will be $U_q(\widehat{\mathfrak{sl}}_2)$. The physical part is in essence defined by two transcendental functions related to the one-point correlators and the two-point neighbour correlators, which depend on physical parameters like temperature, length of the chain, magnetic field, etc.

Later it was discovered [49], that the density matrix can be expressed in terms of fermionic annihilation operators \mathbf{b} and \mathbf{c} , acting on the space of quasi-local operators which act on the states of the chain. By definition quasi-local operators act on an infinite chain but act non-trivially only on a finite segment of the chain. In [50] the corresponding creation operators \mathbf{b}^* and \mathbf{c}^* were constructed along with a bosonic creation operator \mathbf{t}^* . These creation operators generate a basis of the space of quasi-local operators [51], called the fermionic basis. It should be noted that it is not trivially clear that such a construction is possible on an infinite chain. The reason that this is possible is likely the integrable structure of the XXZ chain. In [52] it was explained how to calculate the expectation values of products of the creation operators.

In this work we want to elucidate the construction in [50] and calculate the fermionic operators explicitly on a computer. Using these operators, we want to calculate correlation functions of the XXZ chain. This will be achieved in two ways. First, we will use the exponential form of the density matrix and try to go to bigger lengths as in [53]. Secondly, we want to express local operators in terms of the fermionic basis and use [52] to calculate the corresponding expectation values.

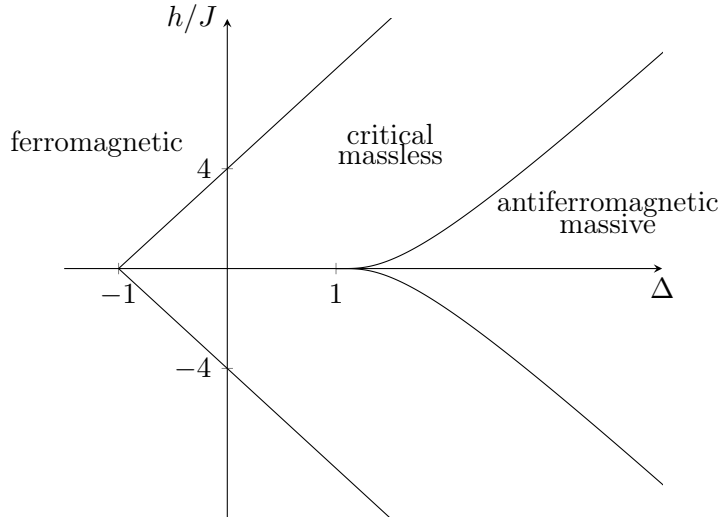
In [50] and [53] the inhomogeneous chain is considered, which entails that every vertical line in the corresponding vertex model is associated with a parameter ξ_j . The monodromy matrix can be represented graphically in this form:

$$a \xrightarrow{\zeta} \begin{array}{c} \uparrow \\ \xi_k | \\ k \end{array} \begin{array}{c} \uparrow \\ \xi_{k+1} | \\ k+1 \end{array} \cdots \begin{array}{c} \uparrow \\ \xi_l | \\ l \end{array} \rightarrow = T_{a,[k,l]}(\zeta) .$$

In past works this approach of introducing inhomogeneities has often proven to be crucial because the additional parameters were needed for regularization. In other works, these parameters were at least convenient because they reduced the order of poles to one. In this work we will explain most of the construction using the inhomogeneities ξ_j for the sake of generality. However, the presented construction does not depend on the inhomogeneities. We will carry out most of the explicit calculations for the homogeneous case, i.e. $\xi_j = 1$. Our hope is that this will be more efficient on a computer since

there are less parameters to handle. The downside of this approach is that we will have to deal with poles of higher order.

In its ground state, the Heisenberg chain has three phases, shown in the following diagram:



We will restrict ourselves to the massless region i.e. $q = e^{i\pi\nu}$ where $\nu \in (0, 1)$ or accordingly $|\Delta| < 1$. Since Δ is invariant under $q \rightarrow q^{-1}$, this covers the whole unit circle. In this work we want to concentrate on the so-called algebraic part which does not depend on physical parameters. This means that most of our work will be valid for all three regions of the diagram. However, to explicitly calculate correlation functions, we will need to solve the physical part of the problem as well. This is done by solving different non-linear integral equations for the different regions (cf. [53, 54]). The restriction to the massless case is done mainly for convenience in order to keep the treatment of the physical part simple. Our second restriction will be that q shall not be a root of unity. It should be noted that the construction can be extended to cover roots of unity, but it is practical to not cover this case from the start.

Let \mathcal{O} be a local operator, meaning that it acts as the identity on the whole chain except for a finite portion. We call $X = q^{2\alpha S(0)}\mathcal{O}$, where $S(k) = \frac{1}{2} \sum_{j=-\infty}^k \sigma_j^z$, a quasi-local operator with tail α . This means that there exist $k \leq l$ such that X acts as $q^{\alpha\sigma_j^z}$ for $j < k$ and as the identity for $j > l$. The length of X is defined as the minimum of $l - k + 1$. The spin of an operator X is defined as its eigenvalue of the operator $\mathbb{S} = [S(\infty), \cdot]$.

Let \mathcal{W}_α be the space of all quasi-local operators with tail α and $\mathcal{W}_{\alpha,s}$ the subspace of those with spin s . We will follow [50] to construct the operators \mathbf{b} , \mathbf{c} , \mathbf{b}^* , \mathbf{c}^* and \mathbf{t}^* acting on

$$\mathcal{W} = \bigoplus_{\alpha \in \mathbb{C}} \mathcal{W}_\alpha . \quad (1.2)$$

These operators have the block structure

$$\begin{aligned} \mathbf{b} &: \mathcal{W}_{\alpha-1,s+1} \rightarrow \mathcal{W}_{\alpha,s} , & \mathbf{c} &: \mathcal{W}_{\alpha+1,s-1} \rightarrow \mathcal{W}_{\alpha,s} , \\ \mathbf{b}^* &: \mathcal{W}_{\alpha+1,s-1} \rightarrow \mathcal{W}_{\alpha,s} , & \mathbf{c}^* &: \mathcal{W}_{\alpha-1,s+1} \rightarrow \mathcal{W}_{\alpha,s} , \\ & & \mathbf{t}^* &: \mathcal{W}_{\alpha,s} \rightarrow \mathcal{W}_{\alpha,s} . \end{aligned}$$

As a first step in our construction we will only consider operators acting on a finite chain in chapter 2. The space of states for a chain segment will be $\mathcal{H}_{[k,l]} = \bigotimes_{j=k}^l V_j$, $V_j \simeq \mathbb{C}^2$, which we will identify with the interval $[k, l]$. If an operator $X \in \text{End } \mathcal{H}_{[j,m]}$ is acting trivially outside the interval $[k, l] \subset [j, m]$ we denote it by $X_{[k,l]}$. Like before the length $\ell(X)$ of an operator X shall be the number of lattice sites in the smallest interval outside of which X acts trivially. We call the corresponding chain segment the support of X .

After constructing all operators in the finite case, we will see that they satisfy so-called reduction relations. These relations will allow us to inductively extend the operators to the infinite chain as the second step in the construction. This will be done in chapter 3 where we also explain how to construct a basis for the space of quasi-local operators \mathcal{W} using the fermionic creation operators in the infinite chain.

Having defined the action of the operators on an infinite chain we will show how to calculate expectation values in chapter 4. Two different techniques will be introduced, both relying on the fermionic operators. In chapter 5 we will explain the implementation of the construction on the computer and in chapter 6 the resulting correlation functions are presented. Finally, in chapter 7, we shall show how both approaches for obtaining expectation values can be connected.

Chapter 2

Operators on the Finite Chain

In this chapter we confine ourselves to operators which act on the finite chain. We will explain the construction of the fermionic operators for this case and then obtain certain reduction relations. Using these relations, we can later define the action of our operators on an infinite chain, which will be covered in the next chapter.

2.1 Basic Definitions

In order to fix the notation, we will give some fundamental definitions in this section. The notation as well as the basic definitions will be very similar to [50] since this is our main reference. Let $V \simeq \mathbb{C}^2$ and $M \simeq \text{End } V$. Now let $V_j \simeq V$ and $M_j \simeq M$ for every $j \in \mathbb{Z}$. The space of states of a segment of the chain is $\mathcal{H}_{[k,l]} = \bigotimes_{j=k}^l V_j$. We will identify such a segment with the corresponding interval $[k, l]$. Furthermore we call the space of operators acting on a segment $[k, l] \subset \mathbb{Z}$

$$M_{[k,l]} = \bigotimes_{j=k}^l M_j . \quad (2.1)$$

For our L operators we will use two auxiliary spaces. On the one hand we will use two-dimensional representations of $U_q(\mathfrak{sl}_2)$. These will be denoted by small Latin characters as indices. On the other hand, we will use representations of the q-oscillator algebra Osc . For these we will use capital Latin indices.

For our first auxiliary space we will write

$$L_{a,j}(\zeta) = \rho(\zeta) L_{a,j}^{\circ}(\zeta) \in M_a \otimes M_j , \quad (2.2)$$

where

$$L_{a,j}^\circ(\zeta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \beta(\zeta) & \gamma(\zeta) & 0 \\ 0 & \gamma(\zeta) & \beta(\zeta) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (2.3)$$

$$\beta(\zeta) = \frac{\zeta - \zeta^{-1}}{q\zeta - q^{-1}\zeta^{-1}}, \quad \gamma(\zeta) = \frac{q - q^{-1}}{q\zeta - q^{-1}\zeta^{-1}}. \quad (2.4)$$

It is easy to prove that

$$L_{a,j}^\circ(\zeta)^{-1} = L_{a,j}^\circ(\zeta^{-1}). \quad (2.5)$$

For the normalization factor $\rho(\zeta)$ see subsection 2.1.1.

Now we want to define L operators for our second auxiliary space. We fix the q -oscillator algebra by giving the following relations for the generators \mathbf{a}, \mathbf{a}^* and $q^{\pm D}$

$$\begin{aligned} q^D \mathbf{a} q^{-D} &= q^{-1} \mathbf{a}, & q^D \mathbf{a}^* q^{-D} &= q \mathbf{a}^* \\ \mathbf{a} \mathbf{a}^* &= 1 - q^{2D+2}, & \mathbf{a}^* \mathbf{a} &= 1 - q^{2D}. \end{aligned} \quad (2.6)$$

The L operator is

$$L_{A,j}(\zeta) = \sigma(\zeta) L_{A,j}^\circ(\zeta) \in Osc_A \otimes M_j, \quad (2.7)$$

where

$$L_{A,j}^\circ(\zeta) = \begin{pmatrix} 1 - \zeta^2 q^{2D_A+2} & -\zeta \mathbf{a}_A \\ -\zeta \mathbf{a}_A^* & 1 \end{pmatrix}_j \begin{pmatrix} q^{-D_A} & 0 \\ 0 & q^{D_A} \end{pmatrix}_j, \quad (2.8)$$

$$L_{A,j}^\circ(\zeta)^{-1} = \frac{1}{1 - \zeta^2} \begin{pmatrix} q^{D_A} & 0 \\ 0 & q^{-D_A} \end{pmatrix}_j \begin{pmatrix} 1 & \zeta \mathbf{a}_A \\ \zeta \mathbf{a}_A^* & 1 - \zeta^2 q^{2D_A} \end{pmatrix}_j. \quad (2.9)$$

As before, see subsection 2.1.1 for the normalization factor $\sigma(\zeta)$.

We say that an operator $X_{[k,l]} \in M_{[k,l]}$ has spin s , if

$$\mathbb{S}(X_{[k,l]}) = s X_{[k,l]}, \quad (2.10)$$

where

$$\mathbb{S}(X_{[k,l]}) = [S_{[k,l]}, X_{[k,l]}], \quad S_{[k,l]} = \frac{1}{2} \sum_{j \in [k,l]} \sigma_j^z. \quad (2.11)$$

By defining it like this, an operator of spin s' will change the spin of a state it acts upon by s' : Suppose $X_{[k,l]} \in M_{[k,l]}$ is of spin s' and $|\psi\rangle \in \mathcal{H}_{[k,l]}$ has spin s . Then

$$S_{[k,l]} X_{[k,l]} |\psi\rangle = (\mathbb{S}(X_{[k,l]}) + X_{[k,l]} S_{[k,l]}) |\psi\rangle = (s + s') X_{[k,l]} |\psi\rangle, \quad (2.12)$$

i.e. $X_{[k,l]} |\psi\rangle$ has spin $s + s'$.

In the following we will consider adjoint actions of operators. These will act on the spaces M_a , Osc_A , $M_{[k,l]}$, etc. and will be denoted by boldface letters $\mathbf{b}, \mathbf{c}, \dots$ or blackboard boldface letters $\mathbb{T}, \mathbb{S}, \dots$. One example is the adjoint action of the L operator

$$\mathbb{L}_{a,j}(\zeta)(X_{[k,l]}) := L_{a,j}(\zeta)X_{[k,l]}L_{a,j}(\zeta)^{-1} \in M_a \otimes M_{[k,l]} . \quad (2.13)$$

Here we use $X_{[k,l]} \in M_a \otimes M_{[k,l]}$, which acts as identity on M_a . This means that $\mathbb{L}_{a,j}(\zeta) \in \text{End } M_a \otimes \text{End } M_{[k,l]}$. Indices are used to indicate the space that an operator is acting on, e.g. $\mathbf{x}_{[k,l]} \in \text{End } M_{[k,l]}$. We will often drop the suffix if an operand is present. If $X_{[k,l]} \in M_{[k,l]}$ it is implied that $\mathbf{x} \in \text{End } M_{[k,l]}$ in $\mathbf{x}(X_{[k,l]})$.

We define the twisted transfer matrix as the trace over the adjoint action of the monodromy matrix

$$T_{a,[k,l]}(\zeta) = L_{a,l}(\zeta/\xi_l) \cdots L_{a,k}(\zeta/\xi_k) , \quad (2.14a)$$

$$\mathbb{T}_a(\zeta, \alpha)(X_{[k,l]}) = T_{a,[k,l]}(\zeta)q^{\alpha\sigma_a^z}X_{[k,l]}T_{a,[k,l]}(\zeta)^{-1} , \quad (2.14b)$$

$$\mathbf{t}^*(\zeta, \alpha)(X_{[k,l]}) = \text{tr}_a [\mathbb{T}_a(\zeta, \alpha)(X_{[k,l]})] . \quad (2.14c)$$

As noted in the introduction we keep the inhomogeneities ξ_j for this part of the construction. The monodromy matrix may also be expressed in terms of the adjoint actions of L operators

$$\mathbb{T}_a(\zeta, \alpha)(X_{[k,l]}) = \mathbb{L}_{a,l}(\zeta/\xi_l) \cdots \mathbb{L}_{a,k}(\zeta/\xi_k)(q^{\alpha\sigma_a^z}X_{[k,l]}) . \quad (2.15)$$

We say that an operator $\mathbf{x}_{[k,l]} \in \text{End } M_{[k,l]}$ has spin s , if

$$[\mathbb{S}, \mathbf{x}_{[k,l]}] = s \mathbf{x}_{[k,l]} . \quad (2.16)$$

We write $s(\mathbf{x}) = s$ if \mathbf{x} has spin s . Analogous to the above definition, if $X_{[k,l]} \in M_{[k,l]}$ has spin s , then $\mathbf{x}(X_{[k,l]}) \in M_{[k,l]}$ has spin $s + s(\mathbf{x})$. To provide an overview we will now list the spins of some operators which will be introduced later:

$$s(\mathbf{x}) = \begin{cases} 0 & \text{if } \mathbf{x} = \mathbf{t}^*, \mathbf{q} \\ 1 & \text{if } \mathbf{x} = \mathbf{k}, \mathbf{f}, \mathbf{c}, \bar{\mathbf{c}}, \mathbf{b}^* \\ -1 & \text{if } \mathbf{x} = \mathbf{b}, \bar{\mathbf{b}}, \mathbf{c}^* \end{cases} . \quad (2.17)$$

Using a representation of Osc_A as auxiliary space we define the \mathbf{q} operator in a similar manner as the twisted transfer matrix

$$T_{A,[k,l]}(\zeta) = L_{A,l}(\zeta/\xi_l) \cdots L_{A,k}(\zeta/\xi_k) , \quad (2.18a)$$

$$\mathbb{T}_A(\zeta, \alpha)(X_{[k,l]}) = T_{A,[k,l]}(\zeta)q^{2\alpha D_A}X_{[k,l]}T_{A,[k,l]}(\zeta)^{-1} , \quad (2.18b)$$

$$\mathbf{q}(\zeta, \alpha)(X_{[k,l]}) = \text{tr}_A \left[\mathbb{T}_A(\zeta, \alpha)\zeta^{\alpha-\mathbb{S}}(q^{-2S_{[k,l]}}X_{[k,l]}) \right] . \quad (2.18c)$$

The factor $\zeta^{\alpha-\mathbb{S}}$ in the definition of $\mathbf{q}_{[k,l]}(\zeta, \alpha)$ results in a very simple tq equation:

$$\mathbf{t}_{[k,l]}^*(\zeta, \alpha)\mathbf{q}_{[k,l]}(\zeta, \alpha) = \mathbf{q}_{[k,l]}(q\zeta, \alpha) + \mathbf{q}_{[k,l]}(q^{-1}\zeta, \alpha) , \quad (2.19)$$

which will be shown in the next section. The reason for introducing the factor $q^{-2\mathbb{S}_{[k,l]}}$ will be explained later.

We then define the spin reversal operator

$$\mathbb{J}(X_{[k,l]}) = \prod_{j \in [k,l]} \sigma_j^x \cdot X_{[k,l]} \cdot \prod_{j \in [k,l]} \sigma_j^x . \quad (2.20)$$

It is easy to see that

$$\mathbb{S} \circ \mathbb{J}(X_{[k,l]}) = -\mathbb{J} \circ \mathbb{S}(X_{[k,l]}) . \quad (2.21)$$

Lastly, we set the transformation

$$\phi_\alpha(\mathbf{x}_{[k,l]}(\zeta, \alpha)) = q^{-1}N(\alpha - \mathbb{S}_{[k,l]} - 1) \circ \mathbb{J}_{[k,l]} \circ \mathbf{x}_{[k,l]}(\zeta, -\alpha) \circ \mathbb{J}_{[k,l]} , \quad (2.22)$$

where

$$N(x) = q^{-x} - q^x ,$$

which will be used later.

2.1.1 Crossing Symmetry

Since [49], [50] and [52] are inspired by conformal field theory (CFT), the authors demand that the L operators obey the crossing symmetry relation

$$L_{\cdot,j}(\zeta)^{-1} = \sigma_j^y L_{\cdot,j}(q^{-1}\zeta)^{t_j} \sigma_j^y . \quad (2.23)$$

We denote by $(\cdot)^{t_j}$ the transposition with respect to the quantum space M_j . This symmetry fixes the normalization factors $\rho(\zeta)$ and $\sigma(\zeta)$ by the two relations

$$\sigma(\zeta)\sigma(q^{-1}\zeta) = \frac{1}{1-\zeta^2} \quad (2.24)$$

and

$$\rho(\zeta)\rho(q^{-1}\zeta) = q^{-1} \frac{1-\zeta^2}{1-q^{-2}\zeta^2} . \quad (2.25)$$

Using both of these relations one can additionally show that

$$\rho(\zeta) = \frac{q^{-1/2}\sigma(q^{-1}\zeta)}{\sigma(\zeta)} . \quad (2.26)$$

These relations are used in the construction of the fused L operator in the next section.

It should be noted however, that the crossing symmetry is not needed for the construction. If crossing symmetry is not demanded, a global factor for the fused operator $L_{\{a,A\},j}(\zeta)$ appears, which does not concern us since we consider adjoint actions. Secondly, the tq equation becomes slightly more complicated.

In this work we shall demand crossing symmetry for the sake of simplicity and to be compatible with the literature.

2.2 Construction of $\mathbf{k}(\zeta, \alpha)$

In this section we will consider the construction of the operator $\mathbf{k}_{[k,l]}$. Most of the operators which will be considered in this work will be derived from $\mathbf{k}_{[k,l]}$. Let us first introduce the fused L operator $L_{\{a,A\},j}$:

$$L_{\{a,A\},j}(\zeta) = F_{a,A}^{-1} L_{a,j}(\zeta) L_{A,j}(\zeta) F_{a,A}, \quad (2.27a)$$

where $F_{a,A} = 1 - \mathbf{a}_A \sigma_a^+$ and thus $F_{a,A}^{-1} = 1 + \mathbf{a}_A \sigma_a^+$. After some calculation it can be brought to a form triangular on M_a :

$$L_{\{a,A\},j}(\zeta) = \begin{pmatrix} 1 & 0 \\ \frac{\gamma(\zeta)}{\beta(\zeta)} \sigma_j^+ & 1 \end{pmatrix}_a \begin{pmatrix} L_{A,j}(q\zeta) q^{-\sigma_j^z/2} & 0 \\ 0 & L_{A,j}(q^{-1}\zeta) q^{\sigma_j^z/2} \end{pmatrix}_a. \quad (2.27b)$$

The corresponding monodromy matrix is therefore also triangular:

$$T_{\{a,A\},[k,l]}(\zeta) = L_{\{a,A\},l}(\zeta/\xi_l) \cdots L_{\{a,A\},k}(\zeta/\xi_k) = \begin{pmatrix} A_{A,[k,l]}(\zeta) & 0 \\ C_{A,[k,l]}(\zeta) & D_{A,[k,l]}(\zeta) \end{pmatrix}_a, \quad (2.28)$$

$$A_{A,[k,l]}(\zeta) = T_{A,[k,l]}(q\zeta) q^{-S_{[k,l]}}, \quad D_{A,[k,l]}(\zeta) = T_{A,[k,l]}(q^{-1}\zeta) q^{S_{[k,l]}}. \quad (2.29)$$

Using that $[F_{a,A}, q^{\alpha\sigma_a^z + 2\alpha D_A}] = 0$ and $q^{\mathbb{S}}(X_{[k,l]}) = q^{S_{[k,l]}} X_{[k,l]} q^{-S_{[k,l]}}$, it can be shown with a short calculation that the adjoint action of the monodromy matrix is also triangular:

$$\mathbb{T}_{\{a,A\}}(\zeta, \alpha)(X_{[k,l]}) = F_{a,A}^{-1} (\mathbb{T}_a(\zeta, \alpha) \mathbb{T}_A(\zeta, \alpha)(X_{[k,l]})) F_{a,A} \quad (2.30a)$$

$$= T_{\{a,A\},[k,l]}(\zeta) q^{\alpha\sigma_a^z} q^{2\alpha D_A} X_{[k,l]} T_{\{a,A\},[k,l]}^{-1}(\zeta) \quad (2.30b)$$

$$= \begin{pmatrix} \mathbb{A}_A(\zeta, \alpha)(X_{[k,l]}) & 0 \\ \mathbb{C}_A(\zeta, \alpha)(X_{[k,l]}) & \mathbb{D}_A(\zeta, \alpha)(X_{[k,l]}) \end{pmatrix}_a, \quad (2.30c)$$

$$\mathbb{A}_A(\zeta, \alpha)(X_{[k,l]}) = \mathbb{T}_A(q\zeta, \alpha) q^{\alpha - \mathbb{S}}(X_{[k,l]}) \quad (2.31a)$$

$$\mathbb{D}_A(\zeta, \alpha)(X_{[k,l]}) = \mathbb{T}_A(q^{-1}\zeta, \alpha) q^{-\alpha + \mathbb{S}}(X_{[k,l]}) . \quad (2.31b)$$

Before going on to defining $\mathbf{k}_{[k,l]}$ we want to show that the tq equation (2.19) can be easily derived from the above expression. This can be done by taking the trace over both auxiliary spaces M_a and Osc_A . Let $X_{[k,l]}$ be an operator of spin s and consider

$$\begin{aligned} & \text{tr}_{a,A} \left\{ F_{a,A}^{-1} (\mathbb{T}_a(\zeta, \alpha) \mathbb{T}_A(\zeta, \alpha) (q^{-2S_{[k,l]}} X_{[k,l]})) F_{a,A} \right\} \\ &= \zeta^{-\alpha+s} \text{tr}_a \left\{ \mathbb{T}_a(\zeta, \alpha) \text{tr}_A \left\{ \mathbb{T}_A(\zeta, \alpha) \zeta^{\alpha-\mathbb{S}} (q^{-2S_{[k,l]}} X_{[k,l]}) \right\} \right\} \\ &= \zeta^{-\alpha+s} \text{tr}_a \left\{ \mathbb{T}_a(\zeta, \alpha) \mathbf{q}(\zeta, \alpha) (X_{[k,l]}) \right\} \\ &= \zeta^{-\alpha+s} \mathbf{t}^*(\zeta, \alpha) \mathbf{q}(\zeta, \alpha) (X_{[k,l]}) \end{aligned}$$

on the one hand and the trace over (2.30c) on the other hand. The latter gives us

$$\begin{aligned} & \text{tr}_A \left\{ \mathbb{A}_A(\zeta, \alpha) (q^{-2S_{[k,l]}} X_{[k,l]}) + \mathbb{D}_A(\zeta, \alpha) (q^{-2S_{[k,l]}} X_{[k,l]}) \right\} \\ &= \zeta^{-\alpha+s} \text{tr}_A \left\{ \mathbb{T}_A(q\zeta, \alpha) (q\zeta)^{\alpha-\mathbb{S}} (q^{-2S_{[k,l]}} X_{[k,l]}) \right. \\ & \quad \left. + \mathbb{T}_A(q^{-1}\zeta, \alpha) (q^{-1}\zeta)^{\alpha-\mathbb{S}} (q^{-2S_{[k,l]}} X_{[k,l]}) \right\} \\ &= \zeta^{-\alpha+s} \left(\mathbf{q}(q\zeta, \alpha) (X_{[k,l]}) + \mathbf{q}(q^{-1}\zeta, \alpha) (X_{[k,l]}) \right), \end{aligned}$$

which then yields the tq equation (2.19) for our adjoint operators.

Apparently, only the diagonal part of $\mathbb{T}_{\{a,A\}}(\zeta, \alpha) (X_{[k,l]})$ is used to derive the tq equation. Now we want to consider the off-diagonal part of $\mathbb{T}_{\{a,A\},[k,l]}(\zeta, \alpha)$. The operator $\mathbf{k}_{[k,l]}(\zeta, \alpha)$ is defined using this off-diagonal part:

$$\mathbf{k}(\zeta, \alpha) (X_{[k,l]}) = \text{tr}_A \left\{ \mathbb{C}_A(\zeta, \alpha) \zeta^{\alpha-\mathbb{S}} (q^{-2S_{[k,l]}} X_{[k,l]}) \right\} \quad (2.32a)$$

$$= \text{tr}_{a,A} \left\{ \sigma_a^+ \mathbb{T}_a(\zeta, \alpha) \mathbb{T}_A(\zeta, \alpha) \zeta^{\alpha-\mathbb{S}} (q^{-2S_{[k,l]}} X_{[k,l]}) \right\}. \quad (2.32b)$$

The operator $\mathbf{k}_{[k,l]}(\zeta, \alpha)$ is used to derive the annihilation operators $\bar{\mathbf{c}}_{[k,l]}(\zeta, \alpha)$, $\mathbf{c}_{[k,l]}(\zeta, \alpha)$ and $\mathbf{f}_{[k,l]}(\zeta, \alpha)$. In order to obtain these, we will need to do a partial fraction decomposition of $\mathbf{k}_{[k,l]}(\zeta, \alpha)$. Before doing this we will explain the analytic structure of $\mathbf{k}_{[k,l]}(\zeta, \alpha)$ in the next section.

2.3 Analytic Structure of $\mathbf{k}(\zeta, \alpha)$, $\mathbf{q}(\zeta, \alpha)$ and $\mathbf{t}^*(\zeta, \alpha)$

In this section we want to explain the analytic structure of $\mathbf{t}_{[k,l]}^*(\zeta, \alpha)$, $\mathbf{q}_{[k,l]}(\zeta, \alpha)$ and $\mathbf{k}_{[k,l]}(\zeta, \alpha)$. This is done in large parts in [50], but since it is important for all following considerations it seems practical to present it here.

An examination of (2.3) and (2.8) gives rise to the idea that $\mathbf{t}_{[k,l]}^*(\zeta, \alpha)$ and $\mathbf{q}_{[k,l]}(\zeta, \alpha)$ are rational in ζ^2 , with possibly an additional factor $\zeta^{-\alpha \pm \mathbb{S}}$.

This is particularly easy to see in the case of $\mathbf{q}_{[k,l]}(\zeta, \alpha)$, since the trace over the auxiliary space is taken and only terms which are “balanced” in \mathbf{a}_A and \mathbf{a}_A^* have a trace not equal to zero. The same argument applies to $\mathbf{t}_{[k,l]}^*(\zeta, \alpha)$, but in a less obvious way. Since we are considering adjoint actions, the factors $\rho(\zeta)$ and $\sigma(\zeta)$ will drop out and therefore do not need to be considered. To examine the analytic structure in a more formal fashion we introduce

$$\begin{aligned}\tilde{L}_{a,j}^\circ(\zeta^2) &= \zeta^{-\sigma_j^z/2} L_{a,j}^\circ(\zeta) \zeta^{\sigma_j^z/2} , \\ \tilde{L}_{A,j}^\circ(\zeta^2) &= \zeta^{-\sigma_j^z/2-1} L_{A,j}^\circ(\zeta) \zeta^{-\sigma_j^z/2} .\end{aligned}$$

Both operators and their inverse operators are rational functions in ζ^2 and regular at $\zeta^2 = \infty$. The operators $\tilde{L}_{a,j}^\circ(\zeta^2)$ and $\tilde{L}_{a,j}^\circ(\zeta^2)^{-1}$ have poles only at $\zeta^2 = q^{-2}$ and $\zeta^2 = q^2$ respectively. The operator $\tilde{L}_{A,j}^\circ(\zeta^2)$ has a pole at $\zeta^2 = 0$ and $\tilde{L}_{A,j}^\circ(\zeta^2)^{-1}$ has one at $\zeta^2 = 1$.

Now denote by $\tilde{\mathbb{T}}_{a,[k,l]}(\zeta^2, \alpha)$ and $\tilde{\mathbb{T}}_{A,[k,l]}(\zeta^2, \alpha)$ the operators $\mathbb{T}_{a,[k,l]}(\zeta, \alpha)$ and $\mathbb{T}_{A,[k,l]}(\zeta, \alpha)$ in which the L operators have been replaced by $\tilde{L}_{a,j}^\circ(\zeta^2)$ and $\tilde{L}_{A,j}^\circ(\zeta^2)$ respectively. These are again rational functions in ζ^2 with poles only at $\zeta^2 = q^{\pm 2} \xi_j^2$ and $\zeta^2 = \xi_j^2$ respectively. Additionally $\tilde{\mathbb{T}}_{A,[k,l]}(\zeta, \alpha)(X_{[k,l]})$ has a pole of order at most s at $\zeta^2 = 0$ if $s > 0$ is the spin of $X_{[k,l]}$. For $s \leq 0$ it is regular at $\zeta^2 = 0$. This can be shown by considering the adjoint action of $\tilde{L}_{A,j}^\circ(\zeta^2)$ on an operator $X_j \in M_j$. $\tilde{L}_{A,j}^\circ(\zeta^2)(X_j)$ has a pole at $\zeta^2 = 0$ only if X_j is of spin 1, i.e. maximal spin. More precisely, one can show by explicit calculation, that $(1 - \zeta^2) \tilde{L}_{A,j}^\circ(\zeta^2)(X_j) = \mathcal{O}(\zeta^{-2s})$. To generalize this to the interval $[k, l]$ and obtain the above statement, it is convenient to represent $X_{[k,l]}$ in terms of the canonical basis $e_{j\alpha}^\beta$, where $e_+^+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $e_-^- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, $e_+^- = \sigma^+$, $e_-^+ = \sigma^-$.

It is easy to prove, that

$$\begin{aligned}\mathbb{T}_a(\zeta, \alpha)(X_{[k,l]}) &= \zeta^{\mathbb{S}} \mathbb{G}^{-1} \tilde{\mathbb{T}}_a(\zeta^2, \alpha) \zeta^{-\mathbb{S}} \mathbb{G}(X_{[k,l]}) , \\ \mathbb{T}_A(\zeta, \alpha)(X_{[k,l]}) &= \zeta^{\mathbb{S}} \mathbb{G}^{-1} \tilde{\mathbb{T}}_A(\zeta^2, \alpha) \zeta^{\mathbb{S}} \mathbb{G}^{-1}(X_{[k,l]}) ,\end{aligned}$$

where $\mathbb{G}(X_{[k,l]}) = G_{[k,l]} X_{[k,l]} G_{[k,l]}^{-1}$ and $G_{[k,l]} = \prod_{j \in [k,l]} \xi_j^{\sigma_j^z/2}$.

By using the first of these relations one can see, that $\mathbf{t}_{[k,l]}^*(\zeta, \alpha)$ is a rational function in ζ^2 with poles at $\zeta^2 = q^{\pm 2} \xi_j^2$. In addition it has to be regular for $\zeta^2 = \infty$. To prove this, one has to write

$$\mathbf{t}^*(\zeta, \alpha)(X_{[k,l]}) = \text{tr}_a \left\{ \zeta^{\mathbb{S}} \mathbb{G}^{-1} \tilde{\mathbb{T}}_a(\zeta^2, \alpha) \zeta^{-\mathbb{S}} \mathbb{G} (\zeta^{\sigma_a^z/2 - \sigma_a^z/2} X_{[k,l]}) \right\}$$

and use that $[L_{a,j}(\zeta, \alpha), \zeta^{\sigma_j^z + \sigma_a^z}] = 0$.

In much the same way one can prove that $\zeta^{-\alpha \pm \mathbb{S}} \mathbf{q}_{[k,l]}(\zeta, \alpha)$ is a rational function in ζ^2 . The poles in $\mathbb{C}^\times = \mathbb{C} \setminus \{0\}$ are at $\zeta^2 = \xi_j^2$ and the operator is

regular for $\zeta^2 = \infty$. At this point it should be noted that the spin s of an operator $X_{[k,l]}$ is always an integer, which explains the sign of S in the factor $\zeta^{-\alpha \pm S}$.

At last we examine the operator $\mathbf{k}_{[k,l]}(\zeta, \alpha)$ from which the annihilation operators are derived. Using the modified monodromy matrices we write it as

$$\mathbf{k}(\zeta, \alpha)(X_{[k,l]}) = \zeta^{\alpha+s+1} \mathbb{G}^{-1} \operatorname{tr}_{a,A} \left\{ \sigma_a^+ \tilde{\mathbb{T}}_a(\zeta^2, \alpha) \tilde{\mathbb{T}}_A(\zeta^2, \alpha) \mathbb{G}^{-1} (q^{-2S_{[k,l]}} X_{[k,l]}) \right\} .$$

If $X_{[k,l]}$ is of spin s , then $\zeta^{-\alpha \pm s - 1} \mathbf{k}(\zeta, \alpha)(X_{[k,l]})$ is a rational function in ζ^2 with poles at $\zeta^2 = \xi_j^2, q^{\pm 2} \xi_j^2$. Moreover $\zeta^{-\alpha - s + 1} \mathbf{k}(\zeta, \alpha)(X_{[k,l]})$ is regular for $\zeta^2 = \infty$. Also $\zeta^{-\alpha - s - 1} \mathbf{k}(\zeta, \alpha)(X_{[k,l]})$ has at most a pole of order s at $\zeta^2 = 0$ if $s > 0$.

2.4 Partial Fraction Decomposition

As mentioned in section 2.2 we need a partial fraction decomposition of the operator $\mathbf{k}_{[k,l]}(\zeta, \alpha)$. Instead of working with $\mathbf{k}_{[k,l]}(\zeta, \alpha)$ directly, it is convenient to introduce

$$\mathbf{k}_{\text{skal}}(\zeta, \alpha)(X_{[k,l]}) = \zeta^{-\alpha - s - 1} \mathbf{k}(\zeta, \alpha)(X_{[k,l]}) . \quad (2.33)$$

From the last section we know that $\mathbf{k}_{\text{skal}}(\zeta, \alpha)$ is rational in ζ^2 and has simple poles at $\zeta^2 = \xi_j^2, q^{\pm 2} \xi_j^2$. Moreover $\mathbf{k}_{\text{skal}}(\zeta, \alpha)$ has no poles at $\zeta^2 = 0$ for $s \leq 0$ and at most a pole of order s in $\zeta^2 = 0$ for $s > 0$. Now we want to define the residues and Laurent coefficients $\rho_j^{(\epsilon)}(\alpha)$ and $\kappa_j(\alpha)$ of $\mathbf{k}_{\text{skal}}(\zeta, \alpha)$. In [53] these are given as

$$\mathbf{k}_{\text{skal}}(\zeta, \alpha)(X_{[k,l]}) = \left[\sum_{j=1}^n \sum_{\epsilon=0,\pm} \frac{\rho_j^{(\epsilon)}(\alpha)}{\zeta^2 - q^{2\epsilon} \xi_j^2} + \sum_{j=1}^s \frac{\kappa_j(\alpha)}{\zeta^{2j}} \right] (X_{[k,l]}) . \quad (2.34)$$

Since we want to consider the homogeneous case, we will need a different decomposition. In the homogeneous case the three series of poles at $\zeta^2 = \xi_j^2, q^{\pm 2} \xi_j^2$ merge into three poles of higher order at $\zeta^2 = 1, q^{\pm 2}$. For $\mathbf{k}_{\text{skal}}(\zeta, \alpha)(X_{[k,l]})$ these poles have order $\ell(X_{[k,l]}) = l - k + 1$. This leads to the decomposition

$$\mathbf{k}_{\text{skal}}(\zeta, \alpha)(X_{[k,l]}) = \left[\sum_{j=1}^n \sum_{\epsilon=0,\pm} \frac{\rho_j^{(\epsilon)}(\alpha)}{(\zeta^2 - q^{2\epsilon})^j} + \sum_{j=1}^s \frac{\kappa_j(\alpha)}{\zeta^{2j}} \right] (X_{[k,l]}) . \quad (2.35)$$

2.5 Construction of $\mathbf{c}(\zeta, \alpha)$, $\mathbf{b}(\zeta, \alpha)$ and $\mathbf{f}(\zeta, \alpha)$

The annihilation operators $\mathbf{c}_{[k,l]}$, $\mathbf{b}_{[k,l]}$ and $\mathbf{f}_{[k,l]}$ are defined through the decomposition of $\mathbf{k}_{[k,l]}$ into its three series of poles:

$$\begin{aligned} \mathbf{k}(\zeta, \alpha)(X_{[k,l]}) &= \\ &(\bar{\mathbf{c}}(\zeta, \alpha) + \mathbf{c}(q\zeta, \alpha) + \mathbf{c}(q^{-1}\zeta, \alpha) + \mathbf{f}(q\zeta, \alpha) - \mathbf{f}(q^{-1}\zeta, \alpha))(X_{[k,l]}) . \end{aligned} \quad (2.36)$$

We demand that the three new operators are similar to $\mathbf{k}_{[k,l]}$ in the sense that for $X_{[k,l]}$ with spin s the operators $\bar{\mathbf{c}}_{[k,l]}(\zeta, \alpha)X_{[k,l]}$, $\mathbf{c}_{[k,l]}(\zeta, \alpha)X_{[k,l]}$ and $\mathbf{f}_{[k,l]}(\zeta, \alpha)X_{[k,l]}$ can be written as $\zeta^{\alpha+s+1}f_{[k,l]}(\zeta^2)$. Here $f_{[k,l]}(\zeta^2)$ shall be rational in ζ^2 and have poles only at $\zeta^2 = \xi_j^2$ ($j \in [k, l]$). This way $\bar{\mathbf{c}}_{[k,l]}(\zeta, \alpha)X_{[k,l]}$ produces the series of poles along the real axis while $\mathbf{c}_{[k,l]}(\zeta, \alpha)X_{[k,l]}$ and $\mathbf{f}_{[k,l]}(\zeta, \alpha)X_{[k,l]}$ produce the other two series. In order to accommodate for the pole at $\zeta^2 = 0$, we will allow \mathbf{f} to have a pole at this point. The decomposition (2.36) is realized by means of the relations

$$\bar{\mathbf{c}}(\zeta, \alpha)(X_{[k,l]}) = \frac{1}{2\pi i} \oint_{\Gamma} \psi(\zeta/\xi, \alpha + s + 1) \mathbf{k}(\xi, \alpha)(X_{[k,l]}) \frac{d\xi^2}{\xi^2} , \quad (2.37)$$

$$\begin{aligned} \mathbf{c}(\zeta, \alpha)(X_{[k,l]}) &= \frac{1}{4\pi i} \\ &\times \oint_{\Gamma} \psi(\zeta/\xi, \alpha + s + 1) \{ \mathbf{k}(q\xi, \alpha) + \mathbf{k}(q^{-1}\xi, \alpha) \} (X_{[k,l]}) \frac{d\xi^2}{\xi^2} , \end{aligned} \quad (2.38)$$

$$\mathbf{f}(\zeta, \alpha)(X_{[k,l]}) = \{ \mathbf{f}^{\text{sing}}(\zeta, \alpha) + \mathbf{f}^{\text{reg}}(\zeta, \alpha) \} (X_{[k,l]}) , \quad (2.39)$$

$$\begin{aligned} \mathbf{f}^{\text{sing}}(\zeta, \alpha)(X_{[k,l]}) &= \frac{1}{4\pi i} \\ &\times \oint_{\Gamma} \psi(\zeta/\xi, \alpha + s + 1) \{ -\mathbf{k}(q\xi, \alpha) + \mathbf{k}(q^{-1}\xi, \alpha) \} (X_{[k,l]}) \frac{d\xi^2}{\xi^2} , \end{aligned} \quad (2.40)$$

where

$$\psi(\zeta, \alpha) = \frac{1}{2} \frac{\zeta^2 + 1}{\zeta^2 - 1} \zeta^\alpha . \quad (2.41)$$

Here Γ is a closed curve such that the poles of the integrands at ξ_j^2 , $j \in [k, l]$, are inside the curve and the other poles $q^{\pm 2}\xi_j^2$, $q^{\pm 4}\xi_j^2$, 0 , ζ^2 outside.

The operator $\mathbf{f}(\zeta, \alpha)$ is split into two parts, namely $\mathbf{f}^{\text{sing}}(\zeta, \alpha)$ and $\mathbf{f}^{\text{reg}}(\zeta, \alpha)$ which accommodates for the pole at $\zeta^2 = 0$.

We can then introduce additional annihilation operators using the transformation ϕ from (2.22):

$$\bar{\mathbf{b}}_{[k,l]}(\zeta, \alpha) := \phi(\bar{\mathbf{c}})_{[k,l]}(\zeta, \alpha) , \quad \mathbf{b}_{[k,l]}(\zeta, \alpha) := \phi(\mathbf{c})_{[k,l]}(\zeta, \alpha) . \quad (2.42)$$

For the next step we want to express the annihilation operators in terms of their residues or Laurent coefficients. This will allow for an efficient

computation on the computer and at the same time provide an expansion into modes. Such an expansion is useful because of certain properties of the modes, which will be explained in detail later on. The expansion can be done by inserting (2.34) into (2.37)–(2.40). Although we want to concentrate on the homogeneous case, we will first provide expansions for the inhomogeneous case for the sake of completeness. These were obtained in [53]:

$$\bar{\mathbf{c}}(\zeta, \alpha)(X_{[k,l]}) = \zeta^{\alpha+s+1} \sum_{j=1}^n \frac{\zeta^2 + \xi_j^2}{\zeta^2 - \xi_j^2} \cdot \frac{\rho_j^{(0)}(\alpha)}{2\xi_j^2} (X_{[k,l]}) , \quad (2.43)$$

$$\mathbf{c}(\zeta, \alpha)(X_{[k,l]}) = \zeta^{\alpha+s+1} \sum_{j=1}^n \sum_{\epsilon=\pm} \frac{\zeta^2 + \xi_j^2}{\zeta^2 - \xi_j^2} \cdot \frac{q^{\epsilon(\alpha+s-1)} \rho_j^{(\epsilon)}(\alpha)}{4\xi_j^2} (X_{[k,l]}) , \quad (2.44)$$

$$\mathbf{f}(\zeta, \alpha)(X_{[k,l]}) = \zeta^{\alpha+s+1} \left[\sum_{j=0}^s \frac{\zeta^{-2j} \kappa_j(\alpha)}{q^{\alpha+s+1-2j} - q^{2j-\alpha-s-1}} \right. \quad (2.45)$$

$$\left. - \sum_{j=1}^n \sum_{\epsilon=\pm} \frac{\zeta^2 + \xi_j^2}{\zeta^2 - \xi_j^2} \cdot \frac{\epsilon q^{\epsilon(\alpha+s-1)} \rho_j^{(\epsilon)}(\alpha)}{4\xi_j^2} \right] (X_{[k,l]}) , \quad (2.46)$$

where

$$\kappa_0 = - \sum_{j=1}^n \sum_{\epsilon=0,\pm} \frac{\rho_j^{(\epsilon)}(\alpha)}{2q^{2\epsilon} \xi_j^2} . \quad (2.47)$$

As mentioned above we want to focus on the homogeneous case, for which the explicit expansion was not worked out in the literature. We will give a mode expansion like the one above for this case, which will be obtained the same way. The relations (2.37)–(2.40) hold for both cases. The difference between the two cases is the insertion of different decompositions for the operator $\mathbf{k}_{\text{skal}}(\zeta, \alpha)$. For the homogeneous case we will of course use (2.35). For all three integrals we have integrands of the form

$$\begin{aligned} & \xi^{-2} \psi(\zeta/\xi, \alpha + s + 1) \mathbf{k}(q^\epsilon \xi, \alpha)(X_{[k,l]}) \\ &= \zeta^{\alpha+s+1} \frac{\zeta^2 + \xi^2}{2\xi^2(\zeta^2 - \xi^2)} q^{\epsilon(\alpha+s+1)} \mathbf{k}_{\text{skal}}(q^\epsilon \xi, \alpha)(X_{[k,l]}) . \end{aligned} \quad (2.48)$$

Using the expansion

$$\frac{\zeta^2 + \xi^2}{2\xi^2(\zeta^2 - \xi^2)} = \frac{1}{2} \sum_{k=0}^{\infty} (-1)^k (\xi^2 - 1)^k + \frac{1}{\zeta^2 - 1} \sum_{k=0}^{\infty} \left(\frac{\xi^2 - 1}{\zeta^2 - 1} \right)^k \quad (2.49)$$

which is valid for $|\xi^2 - 1| < |\zeta^2 - 1|$ and $|\xi^2 - 1| < 1$ we obtain expansions

for the annihilation operators:

$$\bar{\mathbf{c}}(\zeta, \alpha)(X_{[k,l]}) = \zeta^{\alpha+s+1} \sum_{j=0}^n \frac{\bar{c}_j(\alpha)}{(\zeta^2 - 1)^j} (X_{[k,l]}) , \quad (2.50)$$

$$\mathbf{c}(\zeta, \alpha)(X_{[k,l]}) = \zeta^{\alpha+s+1} \sum_{j=0}^n \frac{c_j(\alpha)}{(\zeta^2 - 1)^j} (X_{[k,l]}) , \quad (2.51)$$

$$\begin{aligned} \mathbf{f}(\zeta, \alpha)(X_{[k,l]}) = \\ \zeta^{\alpha+s+1} \left[\sum_{j=0}^n \frac{f_j(\alpha)}{(\zeta^2 - 1)^j} + \sum_{j=0}^s \frac{\kappa_j(\alpha) \zeta^{-2j}}{q^{\alpha+s+1-2j} - q^{2j-\alpha-s-1}} \right] (X_{[k,l]}) . \end{aligned} \quad (2.52)$$

The coefficients for these expansions are

$$\bar{c}_j(\alpha) = \rho_j^{(0)}(\alpha) , \quad j = 1, \dots, n , \quad (2.53a)$$

$$\bar{c}_0(\alpha) = \frac{1}{2} \sum_{j=1}^n (-1)^{j-1} \bar{c}_j(\alpha) , \quad (2.53b)$$

$$c_j(\alpha) = \frac{1}{2} \left(q^{2j-\alpha-s-1} \rho_j^{(-)}(\alpha) + q^{\alpha+s+1-2j} \rho_j^{(+)}(\alpha) \right) , \quad j = 1, \dots, n , \quad (2.54a)$$

$$c_0(\alpha) = \frac{1}{2} \sum_{j=1}^n (-1)^{j-1} c_j(\alpha) , \quad (2.54b)$$

and

$$f_j(\alpha) = \frac{1}{2} \left(q^{2j-\alpha-s-1} \rho_j^{(-)}(\alpha) - q^{\alpha+s+1-2j} \rho_j^{(+)}(\alpha) \right) , \quad j = 1, \dots, n , \quad (2.55a)$$

$$f_0(\alpha) = \frac{1}{2} \sum_{j=1}^n (-1)^{j-1} f_j(\alpha) , \quad (2.55b)$$

$$\kappa_0(\alpha) = \frac{1}{2} \sum_{j=1}^n (-1)^j \sum_{\epsilon=0,\pm} q^{-2\epsilon j} \rho_j^{(\epsilon)}(\alpha) . \quad (2.55c)$$

To clarify this calculation, we want to provide an example. For brevity we choose to do the calculation for $\bar{\mathbf{c}}(\zeta, \alpha)$. Starting from (2.37) we obtain

$$\bar{\mathbf{c}}(\zeta, \alpha)(X_{[k,l]}) = \frac{1}{2\pi i} \oint_{\Gamma} \zeta^{\alpha+s+1} \frac{\zeta^2 + \xi^2}{2\xi^2(\zeta^2 - \xi^2)} \mathbf{k}_{\text{skal}}(\xi, \alpha)(X_{[k,l]}) d\xi^2 , \quad (2.56)$$

where Γ is a small circle around $\xi^2 = 1$. By inserting the two series (2.35) and (2.49) we get

$$\begin{aligned} \bar{\mathbf{c}}(\zeta, \alpha)(X_{[k,l]}) &= \frac{\zeta^{\alpha+s+1}}{2\pi i} \oint_{\Gamma} \sum_{j=1}^n \frac{\rho_j^{(0)}(\alpha)}{(\xi^2 - 1)^j} \\ &\times \left[\frac{1}{2} \sum_{k=0}^{\infty} (-1)^k (\xi^2 - 1)^k + \frac{1}{\zeta^2 - 1} \sum_{k=0}^{\infty} \left(\frac{\xi^2 - 1}{\zeta^2 - 1} \right)^k \right] (X_{[k,l]}) d\xi^2 \end{aligned} \quad (2.57)$$

which leads to

$$\begin{aligned} \bar{\mathbf{c}}(\zeta, \alpha)(X_{[k,l]}) &= \zeta^{\alpha+s+1} \sum_{j=1}^n \left[\frac{(-1)^{j-1}}{2} + \frac{1}{(\zeta^2 - 1)^j} \right] \rho_j^{(0)}(\alpha)(X_{[k,l]}) \\ &= \zeta^{\alpha+s+1} \left[\underbrace{\frac{1}{2} \sum_{j=1}^n (-1)^{j-1} \rho_j^{(0)}(\alpha)}_{:=\bar{\mathbf{c}}_0(\alpha)} + \sum_{j=1}^n \frac{\rho_j^{(0)}(\alpha)}{(\zeta^2 - 1)^j} \right] (X_{[k,l]}) . \end{aligned} \quad (2.58)$$

The last equation clearly gives us the above expansion for $\bar{\mathbf{c}}(\zeta, \alpha)$ along with the coefficients.

One additional point which should be explained in greater detail is how $\mathbf{f}^{\text{reg}}(\zeta, \alpha)$ is fixed. Above we have given the complete expansion for $\mathbf{f}(\zeta, \alpha)$ for easy reference. To obtain this, one derives an expansion for $\mathbf{f}^{\text{sing}}(\zeta, \alpha)$ in the same way as explained above for $\bar{\mathbf{c}}(\zeta, \alpha)$. Doing this yields

$$\mathbf{f}^{\text{sing}}(\zeta, \alpha)(X_{[k,l]}) = \zeta^{\alpha+s+1} \sum_{j=0}^n \frac{f_j(\alpha)}{(\zeta^2 - 1)^j} (X_{[k,l]}) . \quad (2.59)$$

In order to obtain $\mathbf{f}^{\text{reg}}(\zeta, \alpha)$ we use the decomposition (2.36):

$$\begin{aligned} (\mathbf{k}(\zeta, \alpha) - \bar{\mathbf{c}}(\zeta, \alpha) \\ - \mathbf{c}(q\zeta, \alpha) - \mathbf{c}(q^{-1}\zeta, \alpha) - \mathbf{f}^{\text{sing}}(q\zeta, \alpha) + \mathbf{f}^{\text{sing}}(q^{-1}\zeta, \alpha))(X_{[k,l]}) \\ = (\mathbf{f}^{\text{reg}}(q\zeta, \alpha) - \mathbf{f}^{\text{reg}}(q^{-1}\zeta, \alpha))(X_{[k,l]}) . \end{aligned} \quad (2.60)$$

We now have an equation which fixes the “ q -difference” of $\mathbf{f}^{\text{reg}}(\zeta, \alpha)$. We shall denote the q -difference with respect to ζ with the operator Δ_{ζ} :

$$\Delta_{\zeta} f(\zeta) := f(q\zeta) - f(q^{-1}\zeta) . \quad (2.61)$$

It is possible to invert this operator on the space of Laurent polynomials, which is easy to see when applying it to an arbitrary Laurent polynomial:

$$\Delta_{\zeta} \sum_j a_j \zeta^{2j} = \sum_j (q^{2j} - q^{-2j}) a_j \zeta^{2j} . \quad (2.62)$$

This obviously leads to the inverse action

$$\Delta_\zeta^{-1} \sum_j a_j \zeta^{2j} := \sum_j \frac{a_j}{q^{2j} - q^{-2j}} \zeta^{2j} . \quad (2.63)$$

Inserting the expansions for $\mathbf{k}(\zeta, \alpha)$, $\bar{\mathbf{c}}(\zeta, \alpha)$, $\mathbf{c}(\zeta, \alpha)$ and $\mathbf{f}^{\text{sing}}(\zeta, \alpha)$ into (2.60) gives us

$$\begin{aligned} \zeta^{-\alpha-s-1} \Delta_\zeta \mathbf{f}_{[k,l]}^{\text{reg}}(\zeta, \alpha) &= \sum_{j=1}^s \frac{\kappa_j(\alpha)}{\zeta^{2j}} - \bar{\mathbf{c}}_0(\alpha) \\ &\quad - (q^{\alpha+s+1} + q^{-\alpha-s-1}) \mathbf{c}_0(\alpha) - (q^{\alpha+s+1} - q^{-\alpha-s-1}) \mathbf{f}_0(\alpha) \\ &= \sum_{j=1}^s \frac{\kappa_j(\alpha)}{\zeta^{2j}} - \frac{1}{2} \sum_{j=1}^n (-1)^{j-1} \left(\rho_j^{(0)}(\alpha) + q^{2j} \rho_j^{(-)}(\alpha) + q^{-2j} \rho_j^{(+)}(\alpha) \right) . \end{aligned} \quad (2.64)$$

If we make the ansatz

$$\mathbf{f}^{\text{reg}}(\zeta, \alpha) = \zeta^{\alpha+s+1} \sum_j a_j \zeta^{-2j} \quad (2.65)$$

$$\Rightarrow \Delta_\zeta \mathbf{f}^{\text{reg}}(\zeta, \alpha) = \zeta^{\alpha+s+1} \sum_j (q^{\alpha+s+1-2j} - q^{2j-\alpha-s-1}) a_j \zeta^{-2j} \quad (2.66)$$

we obtain

$$a_j = \frac{\kappa_j(\alpha)}{q^{\alpha+s+1-2j} - q^{2j-\alpha-s-1}} , \quad j = 1, \dots, s \quad (2.67)$$

and

$$(q^{\alpha+s+1} - q^{-\alpha-s-1}) a_0 = \frac{1}{2} \sum_{j=1}^n (-1)^j \sum_{\epsilon=0, \pm} q^{-2j\epsilon} \rho_j^{(\epsilon)}(\alpha) =: \kappa_0(\alpha) . \quad (2.68)$$

Now we have

$$\mathbf{f}_{[k,l]}^{\text{reg}}(\zeta, \alpha) = \zeta^{\alpha+s+1} \sum_{j=0}^s \frac{\kappa_j(\alpha) \zeta^{-2j}}{q^{\alpha+s+1-2j} - q^{2j-\alpha-s-1}} . \quad (2.69)$$

After obtaining expansions for $\bar{\mathbf{c}}_{[k,l]}(\zeta, \alpha)$, $\mathbf{c}_{[k,l]}(\zeta, \alpha)$ and $\mathbf{f}_{[k,l]}(\zeta, \alpha)$ we want to derive one for $\mathbf{b}_{[k,l]}(\zeta, \alpha)$. This can be done by inserting (2.51) into (2.42):

$$\mathbf{b}(\zeta, \alpha)(X_{[k,l]}) = \zeta^{-\alpha-s+1} \sum_{j=0}^n \frac{b_j(\alpha)}{(\zeta^2 - 1)^j} (X_{[k,l]}) , \quad (2.70)$$

where

$$b_j(\alpha) = \phi(c_j)(\alpha) \quad (2.71a)$$

$$= -q^{-1} (q^{\alpha-s} - q^{-\alpha+s}) \mathbb{J} c_j(-\alpha) \mathbb{J} . \quad (2.71b)$$

We do not derive the expansion of $\bar{\mathbf{b}}_{[k,l]}(\zeta, \alpha)$ since it is not needed for our work. However, it should be clear that it can be obtained the same way as above.

2.6 Creation Operators

In the following we want to construct the creation operators $\mathbf{t}_{[k,l]}^*$, $\mathbf{b}_{[k,l]}^*$ and $\mathbf{c}_{[k,l]}^*$. For the creation operators the distinction between the inhomogeneous and the homogeneous case is much more involved than for the annihilation operators. In order to keep things simple, we will concentrate on the homogeneous case.

Let us first consider the operator $\mathbf{t}_{[k,l]}^*(\zeta, \alpha)$. As seen in section 2.3 $\mathbf{t}_{[k,l]}^*(\zeta, \alpha)$ is a rational function in ζ^2 which is regular for $\zeta^2 = \infty$ and has poles at $\zeta^2 = q^{\pm 2} \xi_j^2$, which merge into two poles at $\zeta^2 = q^{\pm 2}$ for the homogeneous case. For reasons that will become clear later, we are interested in the mode expansion

$$\mathbf{t}^*(\zeta, \alpha)(X_{[k,l]}) = \sum_{p=1}^{\infty} (\zeta^2 - 1)^{p-1} t_p^*(\alpha)(X_{[k,l]}) . \quad (2.72)$$

The modes $t_p^*(\alpha)$ are easily obtained by calculating $\mathbf{t}_{[k,l]}^*$ with (2.14) and performing a simple Taylor expansion, which takes very little time on a computer. Still, we want to provide some more details on $\mathbf{t}_{[k,l]}^*$.

In contrast to $\mathbf{k}_{\text{skal}}(\zeta, \alpha)$, we know that $\mathbf{t}^*(\zeta, \alpha)$ does not necessarily vanish for $\zeta^2 = \infty$. Using the definition (2.14) one can find its asymptotic behaviour:

$$\mathbf{t}^*(\zeta, \alpha)(X_{[k,l]}) \sim (q^{\alpha+s} + q^{-\alpha-s})(X_{[k,l]}) \quad \text{for } \zeta^2 \rightarrow \infty , \quad (2.73)$$

if $X_{[k,l]}$ has spin s . To prove this, one considers

$$\begin{aligned} \mathbb{L}_{a,j}(\zeta)(q^{\alpha\sigma_a^z} X_{[k,l]}) &\xrightarrow{\zeta^2 \rightarrow \infty} q^{\text{ad}(\sigma_a^z \sigma_j^z / 2 - 1/2)}(q^{\alpha\sigma_a^z} X_{[k,l]}) \\ &= q^{\text{ad}(\sigma_a^z \sigma_j^z / 2)}(q^{\alpha\sigma_a^z} X_{[k,l]}) \end{aligned} \quad (2.74)$$

which leads to

$$\begin{aligned} \mathbb{T}_a(\zeta, \alpha)(X_{[k,l]}) &= \mathbb{L}_{a,l}(\zeta) \cdots \mathbb{L}_{a,k}(\zeta)(q^{\alpha\sigma_a^z} X_{[k,l]}) \\ &\rightarrow q^{\text{ad}(\sigma_a^z \sigma_l^z / 2)} \cdots q^{\text{ad}(\sigma_a^z \sigma_k^z / 2)}(q^{\alpha\sigma_a^z} X_{[k,l]}) \\ &= q^{\alpha\sigma_a^z} q^{\text{ad}(S_{[k,l]}\sigma_a^z)}(X_{[k,l]}) \\ &= q^{\alpha\sigma_a^z} q^{s\sigma_a^z} X_{[k,l]} \\ &= q^{(\alpha+s)\sigma_a^z} X_{[k,l]} . \end{aligned}$$

Knowing the asymptotic behaviour, we can write down the decomposition

$$\mathbf{t}^*(\zeta, \alpha)(X_{[k,l]}) = \left[\sum_{j=1}^n \sum_{\epsilon=\pm} \frac{\tau_j^{(\epsilon)}(\alpha)}{(\zeta^2 - q^{2\epsilon})^j} + q^{\alpha+s} + q^{-\alpha-s} \right] (X_{[k,l]}) . \quad (2.75)$$

Both formulas for $\mathbf{t}^*(\zeta, \alpha)$ will be used later. For the sake of completeness we will give the modes t_p^* in terms of the Laurent coefficients $\tau_j^{(\epsilon)}$:

$$t_1^*(\alpha)(X_{[k,l]}) = \left[\sum_{j=1}^n \sum_{\epsilon=\pm} \frac{\tau_j^{(\epsilon)}(\alpha)}{(1-q^{2\epsilon})^j} + q^{\alpha+s} + q^{-\alpha-s} \right] (X_{[k,l]}), \quad (2.76a)$$

$$t_p^*(\alpha)(X_{[k,l]}) = \sum_{j=1}^n \sum_{\epsilon=\pm} \binom{-j}{p-1} \frac{\tau_j^{(\epsilon)}(\alpha)(X_{[k,l]})}{(1-q^{2\epsilon})^{p+j-1}}, \quad p = 2, 3, \dots \quad (2.76b)$$

Next, we want to consider the creation operators $\mathbf{b}_{[k,l]}^*$ and $\mathbf{c}_{[k,l]}^*$. As with $\mathbf{t}_{[k,l]}^*$ we are interested in the mode expansions

$$\mathbf{b}^*(\zeta, \alpha)(X_{[k,l]}) = \zeta^{\alpha+s+1} \sum_{p=1}^{\infty} (\zeta^2 - 1)^{p-1} b_p^*(\alpha)(X_{[k,l]}), \quad (2.77)$$

$$\mathbf{c}^*(\zeta, \alpha)(X_{[k,l]}) = \zeta^{-\alpha-s+1} \sum_{p=1}^{\infty} (\zeta^2 - 1)^{p-1} c_p^*(\alpha)(X_{[k,l]}). \quad (2.78)$$

The reason will become clear in the next section.

The creation operators $\mathbf{b}_{[k,l]}^*$ and $\mathbf{c}_{[k,l]}^*$ are obtained in terms of $\mathbf{f}_{[k,l]}$ and $\mathbf{t}_{[k,l]}^*$ by a tq -like equation given in [50]:

$$\mathbf{b}^*(\zeta, \alpha)(X_{[k,l]}) = (\mathbf{f}(q\zeta, \alpha) + \mathbf{f}(q^{-1}\zeta, \alpha) - \mathbf{t}^*(\zeta, \alpha)\mathbf{f}(\zeta, \alpha))(X_{[k,l]}), \quad (2.79)$$

$$\mathbf{c}^*(\zeta, \alpha)(X_{[k,l]}) = -\phi(\mathbf{b}^*)(\zeta, \alpha)(X_{[k,l]}). \quad (2.80)$$

Using the Taylor expansion of $\mathbf{t}_{[k,l]}^*$ and (2.52) and (2.77) we obtain a formula for the modes $b_p^*(\alpha)$:

$$\begin{aligned} b_p^*(\alpha)(X_{[k,l]}) = & \left[\sum_{j=0}^n \binom{-j}{p-1} \frac{q^{\alpha+s+p-j} - (-1)^{p+j} q^{j-p-\alpha-s}}{(q-q^{-1})^{p+j-1}} f_j(\alpha) \right. \\ & + \sum_{j=0}^s \binom{-j}{p-1} \frac{q^{\alpha+s+1-2j} + q^{2j-\alpha-s-1}}{q^{\alpha+s+1-2j} - q^{2j-\alpha-s-1}} \kappa_j(\alpha) \\ & \left. - \sum_{j=0}^n t_{p+j}^*(\alpha) f_j(\alpha) - \sum_{j=0}^s \sum_{k=0}^{p-1} \binom{-j}{k} \frac{t_{p-k}^*(\alpha) \kappa_j(\alpha)}{q^{\alpha+s+1-2j} - q^{2j-\alpha-s-1}} \right] (X_{[k,l]}). \end{aligned} \quad (2.81)$$

We can then derive (2.78) as well as the corresponding modes by using ϕ :

$$c_p^*(\alpha) = \phi(b_p^*)(\alpha) \quad (2.82a)$$

$$= q^{-1}(q^{\alpha-s} - q^{-\alpha+s}) \mathbb{J} b_p^*(-\alpha) \mathbb{J}. \quad (2.82b)$$

2.7 Reduction Relations

In this section we will discuss the so-called reduction relations. They describe how the action of operators $\mathbf{x}_{[j,m]}$ reduces to shorter intervals $[k,l]$ on operators of the form $q^{\alpha(\sigma_j^z + \dots + \sigma_{k-1}^z)} X_{[k,l]}$ where $[k,l] \subset [j,m]$ is a proper subset. These relations can be used to define the action of operators on an infinite chain in terms of operators which act on the finite chain. There are two kinds of reduction relations: left ones and right ones. The left reduction relations are trivial in the sense that they follow directly from the symmetry of the universal R Matrix. By contrast the proof of the right reduction relations is much more involved.

2.7.1 Left Reduction

For the left reduction relations it is sufficient to consider the operators $\mathbf{k}_{[k,l]}$ and $\mathbf{t}_{[k,l]}^*$ which obey the following relations:

$$\mathbf{t}_{[k-1,l]}^*(\zeta, \alpha)(q^{\alpha\sigma_{k-1}^z} X_{[k,l]}) = q^{\alpha\sigma_{k-1}^z} \mathbf{t}_{[k,l]}^*(\zeta, \alpha)(X_{[k,l]}) , \quad (2.83)$$

$$\mathbf{k}_{[k-1,l]}(\zeta, \alpha)(q^{(\alpha+1)\sigma_{k-1}^z} X_{[k,l]}) = q^{\alpha\sigma_{k-1}^z} \mathbf{k}_{[k,l]}(\zeta, \alpha)(X_{[k,l]}) . \quad (2.84)$$

These relations follow easily from the gauge symmetry of the R Matrix, $[L_{a,j}(\zeta, \alpha), q^{\sigma_j^z + \sigma_a^z}] = 0$ and $[L_{A,j}(\zeta, \alpha), q^{\sigma_j^z + 2DA}] = 0$, as we will demonstrate for the first relation:

$$\begin{aligned} \mathbf{t}_{[k-1,l]}^*(\zeta, \alpha)(q^{\alpha\sigma_{k-1}^z} X_{[k,l]}) &= \text{tr}_a \left\{ \mathbb{L}_{a,l} \cdots \mathbb{L}_{a,k-1} (q^{\alpha(\sigma_a^z + \sigma_{k-1}^z)} X_{[k,l]}) \right\} \\ &= q^{\alpha\sigma_{k-1}^z} \text{tr}_a \left\{ \mathbb{L}_{a,l} \cdots \mathbb{L}_{a,k} (q^{\alpha\sigma_a^z} \mathbb{L}_{a,k-1} X_{[k,l]}) \right\} \\ &= q^{\alpha\sigma_{k-1}^z} \text{tr}_a \left\{ \mathbb{L}_{a,l} \cdots \mathbb{L}_{a,k} (q^{\alpha\sigma_a^z} X_{[k,l]}) \right\} \\ &= q^{\alpha\sigma_{k-1}^z} \mathbf{t}_{[k,l]}^*(\zeta, \alpha)(X_{[k,l]}) . \end{aligned}$$

The shift of α in the second relation occurs because of the factor $q^{-2S_{[k,l]}}$ in the definition of $\mathbf{k}_{[k,l]}$.

The left reduction relations for the operators $\mathbf{c}, \mathbf{b}, \mathbf{b}^*, \mathbf{c}^*$ follow from (2.84) with (2.38), (2.22), (2.79) and (2.80) respectively. As a consequence, we obtain the left reduction relations

$$\mathbf{x}_{[k-1,l]}(\zeta, \alpha)(q^{(\alpha+s(\mathbf{x}))\sigma_{k-1}^z} X_{[k,l]}) = q^{\alpha\sigma_{k-1}^z} \mathbf{x}_{[k,l]}(\zeta, \alpha)(X_{[k,l]}) \quad (2.85)$$

for the operators $\mathbf{x} = \mathbf{b}, \mathbf{b}^*, \mathbf{c}, \mathbf{c}^*, \mathbf{t}^*$.

We will use these relations to extend the action of the operators $\mathbf{x}_{[k,l]}$ on operators of the form $q^{\alpha(\sigma_j^z + \dots + \sigma_{k-1}^z)} X_{[k,l]}$ to the semi-infinite interval $(-\infty, l]$.

2.7.2 Right Reduction

The right reduction relations are more complicated. The annihilation operators $\mathbf{x} = \mathbf{b}, \mathbf{c}$ do not extend the support of an operator $X_{[k,l]}$ they are acting on to the right:

$$\mathbf{x}_{[k,l+m]}(\zeta, \alpha)(X_{[k,l]}) = \mathbf{x}_{[k,l]}(\zeta, \alpha)(X_{[k,l]}) . \quad (2.86)$$

The proof is given in section 3.5 of [50]. This can be used to extend the action of the annihilation operators to the semi-infinite interval $[k, \infty)$.

By inserting the mode expansions of the annihilation operators (2.51), (2.70) we get

$$\sum_{p=0}^{n+m} \frac{x_{p,[k,l+m]}(\alpha)(X_{[k,l]})}{(\zeta^2 - 1)^p} = \sum_{p=0}^n \frac{x_{p,[k,l]}(\alpha)(X_{[k,l]})}{(\zeta^2 - 1)^p} \quad (2.87)$$

where $x = b, c$ and $n = l - k + 1$ is the length of $X_{[k,l]}$. By comparing the coefficients, we can conclude that

$$x_{p,[k,l+m]}(\alpha)(X_{[k,l]}) = \begin{cases} x_{p,[k,l]}(\alpha)(X_{[k,l]}) & p = 1, \dots, n \\ 0 & p = n + 1, \dots, m . \end{cases} \quad (2.88)$$

This means any operator X is annihilated by x_p if $p > \ell(X)$. This property is the main reason for calling \mathbf{x} annihilation operators.

The creation operators extend the support of an operator $X_{[k,l]}$ they are acting upon indefinitely to the right. This is the reason for doing the mode expansions (2.72), (2.77), (2.78). As we shall see, the modes $x_p, x = b^*, c^*, t^*$ are finite in the sense that they extend the length of an operator $X_{[k,l]}$ at most by p to the right:

$$\ell(x_p X_{[k,l]}) \leq \ell(X_{[k,l]}) + p . \quad (2.89)$$

Right Reduction for t^*

To better understand the modes of the creation operators it makes sense to consider the expansion of t^* as it was done in section 3.4 in [50]. The authors derive an expansion of the form

$$\mathbf{t}_{[k,l+m]}^*(\zeta, \alpha)(X_{[k,l]}) = \sum_{p=1}^m \mathbf{y}_{[k,l+p]}^{(p)}(\zeta, \alpha)(X_{[k,l]}) + \mathbf{z}_{[k,l+m]}^{(m+1)}(\zeta, \alpha)(X_{[k,l]}) . \quad (2.90)$$

The operators $\mathbf{y}_{[k,l+p]}^{(p)}(\zeta, \alpha)$ and $\mathbf{z}_{[k,l+m]}^{(m+1)}(\zeta, \alpha)$ are rational in ζ^2 . Close to $\zeta^2 = 1$ they behave like $\mathbf{y}_{[k,l+p]}^{(p)}(\zeta, \alpha) = \mathcal{O}((\zeta^2 - 1)^{p-1})$ and $\mathbf{z}_{[k,l+m]}^{(m+1)}(\zeta, \alpha) = \mathcal{O}((\zeta^2 - 1)^m)$. Comparing this to the Taylor expansion of \mathbf{t}^* (2.72) we can

conclude that the p th coefficient $t_{p,[k,l+m]}^*(\alpha)$ extends the support at most by p to the right:

$$t_{p,[k,l+m]}^*(\alpha)(X_{[k,l]}) = t_{p,[k,l+p]}^*(\alpha)(X_{[k,l]}) \quad (2.91)$$

for $p = 1, \dots, m-1$. Since the right-hand side of this equation is independent of m , we may extend the action of the modes infinitely to the right:

$$t_{p,[k,\infty]}^*(\alpha)(X_{[k,l]}) = t_{p,[k,l+p]}^*(\alpha)(X_{[k,l]}) . \quad (2.92)$$

Right Reduction for b^* and c^*

The case of the fermionic creation operators is more complicated but combining lemma 3.1 and lemma 3.7 of [50] leads to an expression that is similar to the above:

$$\mathbf{b}_{[k,l+m]}^*(\zeta, \alpha)(X_{[k,l]}) = \sum_{p=1}^m \mathbf{u}_{[k,l+p]}^{(p)}(\zeta, \alpha)(X_{[k,l]}) + \mathbf{v}_{[k,l+m]}^{(m+1)}(\zeta, \alpha)(X_{[k,l]}) , \quad (2.93)$$

where $\mathbf{u}_{[k,l+m]}^{(p)}(\zeta, \alpha)$ and $\mathbf{v}_{[k,l+m]}^{(m+1)}(\zeta, \alpha)$ have the same properties as the operators $\mathbf{y}_{[k,l+p]}^{(p)}(\zeta, \alpha)$ and $\mathbf{z}_{[k,l+m]}^{(m+1)}(\zeta, \alpha)$ above. By comparing with the Taylor expansion (2.77) we obtain

$$b_{p,[k,l+m]}^*(\alpha)(X_{[k,l]}) = b_{p,[k,l+p]}^*(\alpha)(X_{[k,l]}) \quad (2.94)$$

for $m > p$. From this it follows directly by applying ϕ that

$$c_{p,[k,l+m]}^*(\alpha)(X_{[k,l]}) = c_{p,[k,l+p]}^*(\alpha)(X_{[k,l]}) . \quad (2.95)$$

As above we can use these relations to extend the support of the fermionic creation operators infinitely to the right:

$$b_{p,[k,\infty]}^*(\alpha)(X_{[k,l]}) = b_{p,[k,l+p]}^*(\alpha)(X_{[k,l]}) , \quad (2.96a)$$

$$c_{p,[k,\infty]}^*(\alpha)(X_{[k,l]}) = c_{p,[k,l+p]}^*(\alpha)(X_{[k,l]}) . \quad (2.96b)$$

To sum up, we can write

$$x_{p,[k,l+m]}^*(\alpha)(X_{[k,l]}) = x_{p,[k,l+p]}^*(\alpha)(X_{[k,l]}) \quad (2.97)$$

for $m > p$ and $x_p = b_p^*, c_p^*, t_p^*$.

2.8 Shift in α

Up until now the variable α was not used which means it is still at our disposal. We may shift it in such a way that the spin dependence in the mode expansions

of creation and annihilation operators moves from the spectral parameter to the Taylor and Laurent coefficients. For the annihilation operators we obtain from the Laurent expansions (2.51) and (2.70)

$$\mathbf{x}(\zeta, \alpha - s - s(\mathbf{x}))(X_{[k,l]}) = \zeta^{\alpha s(\mathbf{x})} \sum_{j=0}^n \frac{x_p(\alpha - s - s(\mathbf{x}))(X_{[k,l]})}{(\zeta^2 - 1)^j} \quad (2.98)$$

where $\mathbf{x} = \mathbf{b}, \mathbf{c}$ and $s(\mathbf{b}) = -1$, $s(\mathbf{c}) = 1$.

The Taylor expansions (2.72), (2.77) and (2.78) for the creation operators can be written as

$$\mathbf{x}(\zeta, \alpha - s - s(\mathbf{x}))(X_{[k,l]}) = \zeta^{\alpha s(\mathbf{x})} \sum_{p=1}^{\infty} (\zeta^2 - 1)^{p-1} x_p(\alpha - s - s(\mathbf{x}))(X_{[k,l]}) \quad (2.99)$$

where $\mathbf{x} = \mathbf{b}^*, \mathbf{c}^*, \mathbf{t}^*$. Here the spins are $s(\mathbf{b}^*) = 1$, $s(\mathbf{c}^*) = -1$ and $s(\mathbf{t}^*) = 0$.

If we now insert the right reduction relations for the creation operators (2.91), (2.94) and (2.95) we obtain

$$\begin{aligned} \mathbf{x}_{[k,l+m]}(\zeta, \alpha - s - s(\mathbf{x}))(X_{[k,l]}) = \\ \zeta^{\alpha s(\mathbf{x})} \sum_{p=1}^m (\zeta^2 - 1)^{p-1} x_{p,[k,l+p]}(\alpha - s - s(\mathbf{x}))(X_{[k,l]}) + \mathcal{O}((\zeta^2 - 1)^m) \end{aligned} \quad (2.100)$$

for all $m \in \mathbb{N}$, which may be extended infinitely to the right by the inductive limit $m \rightarrow \infty$,

$$\begin{aligned} \mathbf{x}_{[k,\infty]}(\zeta, \alpha - s - s(\mathbf{x}))(X_{[k,l]}) \\ = \zeta^{\alpha s(\mathbf{x})} \sum_{p=1}^{\infty} (\zeta^2 - 1)^{p-1} x_{p,[k,l+p]}(\alpha - s - s(\mathbf{x}))(X_{[k,l]}) \end{aligned} \quad (2.101)$$

where $\mathbf{x} = \mathbf{b}^*, \mathbf{c}^*, \mathbf{t}^*$. Note that each summand is of finite length. The inductive limit will be discussed in greater detail in section 3.1 .

2.8.1 Products of Operators

Using this shift in the variable α means that we must use different shifts for each creation or annihilation operator in products of operators. Consider a product of two operators $\mathbf{x}, \mathbf{y} = \mathbf{b}, \mathbf{c}, \mathbf{b}^*, \mathbf{c}^*, \mathbf{t}^*$ acting on an operator $X_{[k,l]}$. The shifts in α have to be arranged like this:

$$\mathbf{x}(\zeta, \alpha - s - s(\mathbf{y}) - s(\mathbf{x}))\mathbf{y}(\xi, \alpha - s - s(\mathbf{y}))(X_{[k,l]}) . \quad (2.102)$$

This is easy to understand if we remember, that by convention s is the spin of the operator $X_{[k,l]}$, as in the expression $Y := \mathbf{y}(\xi, \alpha - s - s(\mathbf{y}))(X_{[k,l]})$. Now \mathbf{x} acts on Y , which means that s in $\mathbf{x}(\zeta, \alpha - s - s(\mathbf{x}))(Y)$ becomes the spin of Y , which is $s + s(\mathbf{y})$.

2.9 Commutation Relations

The commutation relations of operators acting on the finite chain are discussed in section 4 of [50]. There they are given in terms of so-called q -exact forms. In the context of [50] a q -exact form is an operator of the form $\mathbf{g}_{[k,l]}(\zeta, \alpha) = \Delta_\zeta \mathbf{h}_{[k,l]}(\zeta, \alpha)$ if $\mathbf{h}_{[k,l]}(\zeta, \alpha) = \zeta^{\alpha+\mathbb{S}}(f_{[k,l]}(\zeta^2))$ where $f_{[k,l]}(\zeta^2)$ is rational in ζ^2 and only has poles in \mathbb{C}^\times at $\zeta^2 = \xi_j^2$ for $j \in [k, l]$. In the homogeneous case this means that it will have a pole only at $\zeta^2 = 1$. As defined before Δ_ζ is the q -difference operator. In analogy to differential calculus $\oint_C \mathbf{g}_{[k,l]}(\zeta, \alpha) \frac{d\zeta^2}{\zeta^2} = 0$ for a cycle C which encloses $\zeta^2 = 1$ but not $\zeta^2 = 0, q^{\pm 2}\zeta^2$. An example for a commutation relation is given in equation (4.3) in [50] which is the relation for the operators \mathbf{t}^* and \mathbf{k} where $k \leq m < l$:

$$\mathbf{k}_{[k,l]}(\xi, \alpha) \mathbf{t}^*(\zeta, \alpha + 1)(X_{[k,m]}) \simeq_\xi \mathbf{t}_{[k,l]}^*(\zeta, \alpha) \mathbf{k}(\xi, \alpha)(X_{[k,m]}) \pmod{(\zeta^2 - 1)^{l-m}}. \quad (2.103)$$

Here ‘ \simeq_ξ ’ means equality up to a q -exact form in ξ . For the construction on the computer it will be important that we have only equality modulo a power of $(\zeta^2 - 1)$. We can obtain the commutation relation for the modes of operators by inserting the Taylor expansions and comparing coefficients. These relations will only hold for t_p^* if $p \leq l - m$, meaning that we may extend the support of the operator $X_{[k,m]}$ at most to the interval $[k, l]$ on which $\mathbf{k}_{[k,l]}$ is defined.

In the following section we will use different shifts for α . This is done for convenience. Since α is a free parameter, we can introduce shifts in order to shorten the following equations.

From this example we can derive the commutation relations for \mathbf{t}^* with \mathbf{c} and \mathbf{b} . The derivation we provide is an additional explanation to the proof of Corollary (4.2) in [50]. To obtain the relation for \mathbf{c} we consider

$$\begin{aligned} & (\mathbf{k}_{[k,l]}(q\xi, \alpha) + \mathbf{k}_{[k,l]}(q^{-1}\xi, \alpha)) \mathbf{t}^*(\zeta, \alpha + 1)(X_{[k,m]}) \\ & \quad - \mathbf{t}_{[k,l]}^*(\zeta, \alpha) (\mathbf{k}(q\xi, \alpha) + \mathbf{k}(q^{-1}\xi, \alpha)) (X_{[k,m]}) \\ & = \Delta_\xi (q\xi)^{\alpha+\mathbb{S}} (f((q\xi)^2)) + \Delta_\xi (q^{-1}\xi)^{\alpha+\mathbb{S}} (f((q^{-1}\xi)^2)) \pmod{(\zeta^2 - 1)^{l-m}} \\ & = (q^2\xi)^{\alpha+\mathbb{S}} (f(q^4\xi^2)) - (q^{-2}\xi)^{\alpha+\mathbb{S}} (f(q^{-4}\xi^2)) \pmod{(\zeta^2 - 1)^{l-m}}. \end{aligned}$$

If we now multiply by $\psi(\zeta/\xi, \alpha + s + 1)/(4\pi i \xi^2)$, integrate and use the definition of \mathbf{c} (2.38), the right-hand side vanishes and we obtain

$$\mathbf{c}_{[k,l]}(\xi, \alpha) \mathbf{t}^*(\zeta, \alpha + 1)(X_{[k,m]}) - \mathbf{t}_{[k,l]}^*(\zeta, \alpha) \mathbf{c}(\xi, \alpha)(X_{[k,m]}) = 0 \pmod{(\zeta^2 - 1)^{l-m}}. \quad (2.104)$$

Because \mathbf{t}^* has spin $s(\mathbf{t}^*) = 0$ and is invariant under spin reversal coupled with changing α to $-\alpha$:

$$\mathbb{J}_{[k,l]} \circ \mathbf{t}_{[k,l]}^*(\zeta, -\alpha) \circ \mathbb{J}_{[k,l]} = \mathbf{t}_{[k,l]}^*(\zeta, \alpha), \quad (2.105)$$

we can obtain the corresponding commutation relation for \mathbf{b} by applying ϕ :

$$\begin{aligned}\phi(\mathbf{t}^*(\zeta, \alpha)\mathbf{c}(\xi, \alpha)) &= q^{-1}N(\alpha - \mathbb{S} - 1)\mathbb{J}\mathbf{t}^*(\zeta, -\alpha)\mathbf{c}(\xi, -\alpha)\mathbb{J} \\ &= \mathbf{t}^*(\zeta, \alpha)q^{-1}N(\alpha - \mathbb{S} - 1)\mathbb{J}\mathbf{c}(\xi, -\alpha)\mathbb{J} \\ &= \mathbf{t}^*(\zeta, \alpha)\mathbf{b}(\xi, \alpha) ,\end{aligned}$$

$$\phi(\mathbf{c}(\xi, \alpha)\mathbf{t}^*(\zeta, \alpha + 1)) = \mathbf{b}(\xi, \alpha)\mathbf{t}^*(\zeta, \alpha - 1) ,$$

which leads directly to

$$\begin{aligned}\mathbf{b}_{[k,l]}(\xi, \alpha)\mathbf{t}^*(\zeta, \alpha - 1)(X_{[k,m]}) - \mathbf{t}_{[k,l]}^*(\zeta, \alpha)\mathbf{b}(\xi, \alpha)(X_{[k,m]}) \\ = 0 \pmod{(\zeta^2 - 1)^{l-m}} .\end{aligned}\quad (2.106)$$

The proofs for most of the commutation relations are extremely complicated and are given in section 4 of [50]. Here we will just provide an overview for the finite and homogeneous case and give some additional remarks. Let us first sum up all commutation relations. All operators commute with \mathbf{t}^* :

$$[\mathbf{c}(\zeta), \mathbf{t}^*(\zeta')] = 0 , \quad [\mathbf{b}(\zeta), \mathbf{t}^*(\zeta')] = 0 , \quad (2.107a)$$

$$[\mathbf{c}^*(\zeta), \mathbf{t}^*(\zeta')] = 0 , \quad [\mathbf{b}^*(\zeta), \mathbf{t}^*(\zeta')] = 0 , \quad (2.107b)$$

$$[\mathbf{t}^*(\zeta), \mathbf{t}^*(\zeta')] = 0 . \quad (2.107c)$$

The remaining operators obey the anticommutation relations

$$[\mathbf{c}(\zeta), \mathbf{c}(\zeta')]_+ = 0 , \quad [\mathbf{b}(\zeta), \mathbf{b}(\zeta')]_+ = 0 , \quad [\mathbf{c}(\zeta), \mathbf{b}(\zeta')]_+ = 0 , \quad (2.108a)$$

$$[\mathbf{c}^*(\zeta), \mathbf{c}^*(\zeta')]_+ = 0 , \quad [\mathbf{b}^*(\zeta), \mathbf{b}^*(\zeta')]_+ = 0 , \quad [\mathbf{c}^*(\zeta), \mathbf{b}^*(\zeta')]_+ = 0 , \quad (2.108b)$$

$$[\mathbf{b}^*(\zeta), \mathbf{c}(\zeta')]_+ = 0 , \quad [\mathbf{c}^*(\zeta), \mathbf{b}(\zeta')]_+ = 0 , \quad (2.108c)$$

$$[\mathbf{b}^*(\zeta), \mathbf{b}(\zeta')]_+ = -\psi(\zeta/\zeta', \alpha) , \quad [\mathbf{c}^*(\zeta), \mathbf{c}(\zeta')]_+ = -\psi(\zeta/\zeta', -\alpha) . \quad (2.108d)$$

The commutation relations which are explicitly proven in [50] are

$$[\mathbf{c}(\zeta), \mathbf{t}^*(\zeta')] = 0 , \quad [\mathbf{b}^*(\zeta), \mathbf{t}^*(\zeta')] = 0 ,$$

$$[\mathbf{c}(\zeta), \mathbf{c}(\zeta')]_+ = 0 , \quad [\mathbf{c}(\zeta), \mathbf{b}(\zeta')]_+ = 0 ,$$

$$[\mathbf{b}^*(\zeta), \mathbf{c}(\zeta')]_+ = 0 , \quad [\mathbf{b}^*(\zeta), \mathbf{b}(\zeta')]_+ = -\psi(\zeta/\zeta', \alpha) .$$

We will show that the rest of the relations except for (2.107c) and the first two equations of (2.108b) follow easily from these. But first we want to note that the commutation relation (2.107c) for the transfer matrix follows directly from the properties of the universal R matrix, namely the Yang-Baxter equation. The first two anticommutation relations of (2.108b) between the creation operators are shown in the separate publication [55].

The last commutation relation for the annihilation operators can be easily derived by applying ϕ to a known relation and multiplying with the factor $N(\alpha - \mathbb{S} + 1)$:

$$N(\alpha - \mathbb{S} + 1)\phi([\mathbf{c}(\zeta), \mathbf{c}(\zeta')]_+) = [\mathbf{b}(\zeta), \mathbf{b}(\zeta')]_+ .$$

In much the same way we can show that $\mathbf{c}^*(\zeta)$ and $\mathbf{b}(\zeta')$ anticommute:

$$-N(\alpha - \mathbb{S} + 1)\phi([\mathbf{b}^*(\zeta), \mathbf{c}(\zeta')]_+) = [\mathbf{c}^*(\zeta), \mathbf{b}(\zeta')]_+ .$$

The commutativity of $\mathbf{t}^*(\zeta)$ with $\mathbf{b}(\zeta')$ has already been shown above and the commutativity with $\mathbf{c}^*(\zeta')$ can be easily shown, too:

$$-N(\alpha - \mathbb{S})\mathbb{J}[\mathbf{b}^*(\zeta), \mathbf{t}^*(\zeta')]\mathbb{J} = [\mathbf{c}^*(\zeta), \mathbf{t}^*(\zeta')] .$$

Finally the only relation left is between $\mathbf{c}^*(\zeta)$ and $\mathbf{c}(\zeta')$ which we will quickly derive from the second equation in (2.108d). Consider

$$\begin{aligned} \mathbf{b}^*(\zeta, \alpha)\mathbf{b}(\xi, \alpha + 1) &= \mathbf{b}^*(\zeta, \alpha)\phi(\mathbf{c}(\xi, \alpha + 1)) \\ &= \mathbf{b}^*(\zeta, \alpha)q^{-1}N(\alpha - \mathbb{S})\mathbb{J}\mathbf{c}(\xi, -\alpha - 1)\mathbb{J} \\ &= q^{-1}N(\alpha - \mathbb{S} + 1)\mathbb{J}\mathbb{J}\mathbf{b}^*(\zeta, \alpha)\mathbb{J}\mathbf{c}(\xi, -\alpha - 1)\mathbb{J} \\ &= \mathbb{J}q^{-1}N(\alpha + \mathbb{S} + 1)\mathbb{J}\mathbf{b}^*(\zeta, \alpha)\mathbb{J}\mathbf{c}(\xi, -\alpha - 1)\mathbb{J} . \end{aligned}$$

Together with $N(-x) = -N(x)$ this leads to

$$\begin{aligned} \mathbb{J}\mathbf{b}^*(\zeta, -\alpha)\mathbf{b}(\xi, -\alpha + 1)\mathbb{J} &= -q^{-1}N(\alpha - \mathbb{S} - 1)\mathbb{J}\mathbf{b}^*(\zeta, -\alpha)\mathbb{J}\mathbf{c}(\xi, \alpha - 1) \\ &= \mathbf{c}^*(\zeta, \alpha)\mathbf{c}(\xi, \alpha - 1) . \end{aligned}$$

In the same way we can get

$$\mathbb{J}\mathbf{b}(\xi, -\alpha)\mathbf{b}^*(\zeta, -\alpha - 1)\mathbb{J} = \mathbf{c}(\xi, \alpha)\mathbf{c}^*(\zeta, \alpha + 1) .$$

This shows that we can obtain the second equation in (2.108d) from the first by changing $\alpha \rightarrow -\alpha$ and reversing the spin.

Chapter 3

Operators on the Infinite Chain

3.1 Inductive Limit

Up to this section we considered operators $X_{[k,l]} \in M_{[k,l]}$ acting on a finite portion of the infinite Heisenberg chain. We constructed several operators $\mathbf{x} \in \text{End } M_{[k,l]}$ acting on these $X_{[k,l]}$ as $\mathbf{x}(X_{[k,l]}) = \mathbf{x}_{[k,l]}(X_{[k,l]})$, meaning that they are of finite length as well.

Following reference [50] we want to define operators corresponding to the \mathbf{x} acting on the whole Heisenberg chain. For this we will use the reduction relations discussed in section 2.7. In order to achieve this, we shall first introduce the so-called quasi-local operators in the following section.

3.1.1 Quasi-Local Operators

We call operators $X_{[k,l]} \in M_{[k,l]}$ local operators, because they act as the identity outside of the interval $[k, l]$. Let

$$S(k) = \frac{1}{2} \sum_{j=-\infty}^k \sigma_j^z \quad (3.1)$$

and \mathbb{S} be the adjoint action. We now call

$$X = q^{2\alpha S(k-1)} X_{[k,l]} \quad (3.2)$$

a quasi-local operator with tail α . As before we say that X has support $[k, l]$ and length $\ell(X) = l - k + 1$. We could also say that an operator is quasi-local if there exists $k \leq l$ such that X acts as $q^{\alpha\sigma_j^z}$ for $j < k$ and as the identity for $j > l$. In this case the length of X would be the minimum of $l - k + 1$.

We denote by \mathcal{W}_α the space spanned by all quasi-local operators with tail α and by $\mathcal{W}_{\alpha,s} \subset \mathcal{W}_\alpha$ the subspace of operators of spin s .

We already know that the creation and annihilation operators change the spin and accordingly shift α . It will become clear that this structure

extends to the operators which act on the infinite chain, giving them the block structure

$$\begin{aligned} \mathbf{b} &: \mathcal{W}_{\alpha-1,s+1} \rightarrow \mathcal{W}_{\alpha,s} , & \mathbf{c} &: \mathcal{W}_{\alpha+1,s-1} \rightarrow \mathcal{W}_{\alpha,s} , \\ \mathbf{b}^* &: \mathcal{W}_{\alpha+1,s-1} \rightarrow \mathcal{W}_{\alpha,s} , & \mathbf{c}^* &: \mathcal{W}_{\alpha-1,s+1} \rightarrow \mathcal{W}_{\alpha,s} , \\ & & \mathbf{t}^* &: \mathcal{W}_{\alpha,s} \rightarrow \mathcal{W}_{\alpha,s} . \end{aligned}$$

This means that our quasi-local operators act on the space

$$\mathcal{W}^{(\alpha)} = \bigoplus_{s=-\infty}^{\infty} \mathcal{W}_{\alpha-s,s} , \quad (3.3)$$

where we may consider $\alpha \in \mathbb{C} \setminus \{0\}$ as a fixed parameter.

3.1.2 Annihilation Operators

We will start with the relatively easy annihilation operators $\mathbf{x} = \mathbf{c}, \mathbf{b}$. For these we found the left and right reduction relations (2.85),(2.86). The right reduction relation allows us to directly extend the support of \mathbf{x} indefinitely to the right:

$$\mathbf{x}_{[k,\infty)}(\zeta, \alpha - s(\mathbf{x}))(X_{[k,l]}) = \mathbf{x}_{[k,l]}(\zeta, \alpha - s(\mathbf{x}))(X_{[k,l]}) . \quad (3.4)$$

Here we use $X_{[k,l]} \in \mathcal{W}^{(\alpha)}$ but the extension to the right would also be possible for a local operator $X_{[k,l]} \in M_{[k,l]}$.

For the extension to the left on the other hand it is important to act on quasi-local operators. For $X_{[k,l]} \in M_{[k,l]}$ we find

$$\begin{aligned} \mathbf{x}_{(-\infty,l]}(\zeta, \alpha - s(\mathbf{x}))(q^{2\alpha S(k-1)} X_{[k,l]}) \\ = q^{2(\alpha-s(\mathbf{x}))S(k-1)} \mathbf{x}_{[k,l]}(\zeta, \alpha - s(\mathbf{x}))(X_{[k,l]}) . \end{aligned} \quad (3.5)$$

Combining these relations allows us to extend the support of an operator $\mathbf{x} = \mathbf{c}, \mathbf{b}$ to the infinite chain. In other words, we can define the action of an operator acting on the infinite chain in terms of finite operators.

We now want to define the action of an operator $\mathbf{x} \in \text{End } \mathcal{W}^{(\alpha)}$ on a quasi-local operator $X \in \mathcal{W}^{(\alpha)}$. To do this we decompose X into quasi-local operators $X^{(s)}$ of spin s :

$$X = \sum_{s=-n}^n X^{(s)} , \quad \mathbb{S}(X^{(s)}) = sX^{(s)} . \quad (3.6)$$

Here we use $n = \ell(X)$. For finite length the spin of an operator is confined

to $-n \leq s \leq n$. Then we can define

$$\begin{aligned}
\mathbf{x}(\zeta)(X) &= \sum_{s=-n}^n \mathbf{x}(\zeta) \left(X^{(s)} \right) \\
&= \sum_{s=-n}^n \mathbf{x}_{(-\infty, \infty)}(\zeta, \alpha - s - s(\mathbf{x})) \left(q^{2(\alpha-s)S(k-1)} X_{[k,l]}^{(s)} \right) \\
&= \sum_{s=-n}^n q^{2(\alpha-s-s(\mathbf{x}))S(k-1)} \mathbf{x}_{[k,l]}(\zeta, \alpha - s - s(\mathbf{x})) \left(X_{[k,l]}^{(s)} \right) . \quad (3.7)
\end{aligned}$$

So, we define the action on an infinite chain in terms of the previously constructed finite operators.

Note that we write $\mathbf{x}(\zeta)$ for an operator acting on the infinite chain and $\mathbf{x}(\zeta, \alpha)$ for an operator acting on the finite chain. We will continue to distinguish finite and infinite operators in this way. The reason for this notation is that for the finite case α is a free variable, whereas in the infinite case it is a fixed parameter specifying the space $\mathcal{W}^{(\alpha)}$ we act upon.

We now want to define the modes for the operators $\mathbf{x}(\zeta)$. Using the previously derived expansions for the annihilation operators we obtain

$$\begin{aligned}
\mathbf{x}(\zeta) \left(X^{(s)} \right) &= q^{2(\alpha-s-s(\mathbf{x}))S(k-1)} \mathbf{x}(\zeta, \alpha - s - s(\mathbf{x})) \left(X_{[k,l]}^{(s)} \right) \\
&= \zeta^{\alpha s(\mathbf{x})} \sum_{j=0}^n \frac{q^{2(\alpha-s-s(\mathbf{x}))S(k-1)} x_j(\alpha - s - s(\mathbf{x}))}{(\zeta^2 - 1)^j} \left(X_{[k,l]}^{(s)} \right)
\end{aligned}$$

where again $n = \ell \left(X_{[k,l]}^{(s)} \right)$. Thus we define

$$\mathbf{x}_p \left(X^{(s)} \right) = \begin{cases} q^{2(\alpha-s-s(\mathbf{x}))S(k-1)} x_p(\alpha - s - s(\mathbf{x})) \left(X_{[k,l]}^{(s)} \right) & p = 0, \dots, n \\ 0 & p > n \end{cases} \quad (3.8)$$

and obtain a Laurent expansion of the operators $\mathbf{x}(\zeta)$ acting on the infinite chain:

$$\mathbf{x}(\zeta) = \zeta^{\alpha s(\mathbf{x})} \sum_{p=0}^{\infty} \frac{\mathbf{x}_p}{(\zeta^2 - 1)^p} . \quad (3.9)$$

From this it follows per definition, that

$$\mathbf{x}_p(X) = 0 \quad \text{for } p > \ell(X) , \quad (3.10)$$

as for the finite case.

3.1.3 Creation Operators

Now we will define the action of the creation operators $\mathbf{x} = \mathbf{b}^*, \mathbf{c}^*, \mathbf{t}^*$ on the infinite chain. For the creation operators we use the same left reduction

relation as for the annihilators (2.85). This means that (3.5) is valid for the creation operators as well. For the right reduction we need to treat the creation operators differently from the annihilation operators. The reason is that the creation operators enlarge the support of the operator they are acting on. As we have seen in section 2.7 each mode \mathbf{x}_p of a creation operator can extend the support by p to the right. This means that the creation operators themselves enlarge the support indefinitely to the right. An expansion to the right was already given by (2.97) for the modes and by (2.101) for the operators themselves. Both relations also hold for operators $X_{[k,l]} \in \mathcal{W}^{(\alpha)}$. Since it is our goal to define the action of the creation operators on the infinite chain in terms of finite operators, we write

$$\begin{aligned} & \mathbf{x}_{[k,\infty)}(\zeta, \alpha - s - s(\mathbf{x}))(X_{[k,l]}) \\ &= \mathbf{x}_{[k,l+m]}(\zeta, \alpha - s - s(\mathbf{x}))(X_{[k,l]}) \pmod{(\zeta^2 - 1)^m}. \end{aligned} \quad (3.11)$$

As for the annihilation operators we now want to obtain an expansion for the creation operators. Let $X^{(s)} \in \mathcal{W}_{\alpha-s,s}$ and $X_{[k,l]}^{(s)} \in M_{[k,l]}$, then

$$\begin{aligned} & \mathbf{x}(\zeta) \left(X^{(s)} \right) \\ &= q^{2(\alpha-s-s(\mathbf{x}))S(k-1)} \mathbf{x}_{[k,l+m]}(\zeta, \alpha - s - s(\mathbf{x})) \left(X_{[k,l]}^{(s)} \right) \pmod{(\zeta^2 - 1)^m} \\ &= \zeta^{\alpha s(\mathbf{x})} \sum_{p=1}^m (\zeta^2 - 1)^{p-1} q^{2(\alpha-s-s(\mathbf{x}))S(k-1)} x_{p,[k,l+p]}(\alpha - s - s(\mathbf{x})) \left(X_{[k,l]} \right) \\ & \pmod{(\zeta^2 - 1)^m}. \end{aligned} \quad (3.12)$$

In the limit $m \rightarrow \infty$ this gives us an expansion

$$\mathbf{x}(\zeta) = \zeta^{\alpha s(\mathbf{x})} \sum_{p=1}^{\infty} (\zeta^2 - 1)^{p-1} \tilde{\mathbf{x}}_p \quad (3.13)$$

where

$$\tilde{\mathbf{x}}_p \left(X^{(s)} \right) = q^{2(\alpha-s-s(\mathbf{x}))S(k-1)} x_{p,[k,l+p]}(\alpha - s - s(\mathbf{x})) \left(X_{[k,l]}^{(s)} \right). \quad (3.14)$$

We will use this expansion only for the bosonic creation operator \mathbf{t}^* . The reason is that the coefficients $\tilde{\mathbf{x}}_p$ of the fermionic operators $\mathbf{b}^*, \mathbf{c}^*$ do not satisfy easy anticommutation relations. For the fermionic operators we will instead introduce the expansion

$$\mathbf{x}(\zeta) = \zeta^{\alpha s(\mathbf{x})+2} \sum_{p=1}^{\infty} (\zeta^2 - 1)^{p-1} \mathbf{x}_p. \quad (3.15)$$

As we will see in the next section the modes \mathbf{x}_p will satisfy the desired anticommutation relations. Note that there is a typo in [50] where the authors wrote -2 instead of $+2$ in the expansion of \mathbf{c}^* .

We calculate the modes \mathbf{x}_p using

$$\zeta^{-2} = \sum_{k=0}^{\infty} (-1)^k (\zeta^2 - 1)^k, \quad |\zeta^2 - 1| < 1.$$

Inserting this in (3.13) we get

$$\begin{aligned} \mathbf{x}(\zeta) &= \zeta^{\alpha s(\mathbf{x})+2} \sum_{p=1}^{\infty} \sum_{k=0}^{\infty} (\zeta^2 - 1)^{p+k-1} (-1)^k \tilde{\mathbf{x}}_p \\ &= \zeta^{\alpha s(\mathbf{x})+2} \sum_{m=1}^{\infty} \sum_{k=0}^{m-1} (\zeta^2 - 1)^{m-1} (-1)^k \tilde{\mathbf{x}}_{m-k} \\ &= \zeta^{\alpha s(\mathbf{x})+2} \sum_{m=1}^{\infty} (\zeta^2 - 1)^{m-1} \sum_{l=1}^m (-1)^{m-l} \tilde{\mathbf{x}}_l \end{aligned} \quad (3.16)$$

which gives us the modes

$$\mathbf{x}_p = \sum_{k=1}^p (-1)^{p-k} \tilde{\mathbf{x}}_k \quad (3.17)$$

for $\mathbf{x} = \mathbf{b}^*, \mathbf{c}^*$.

3.1.4 Commutation Relations of Modes

In section 2.9 we discussed the various commutation relations and anticommutation relations (2.107), (2.108) which our operators obey. These relations are also valid for the new operators acting on $\mathcal{W}^{(\alpha)}$.

We now want to derive commutation relations for the modes $\mathbf{x}_p \in \text{End } \mathcal{W}^{(\alpha)}$ acting on the infinite chain. Most of these relations are very easy to show. We will provide a quick example for the modes \mathbf{c}_p . Let $\mathbf{c}(\zeta) \in \text{End } \mathcal{W}^{(\alpha)}$, then

$$[\mathbf{c}(\zeta), \mathbf{c}(\xi)]_+ = (\zeta\xi)^\alpha \sum_{k,l=0}^{\infty} \frac{[\mathbf{c}_k, \mathbf{c}_l]_+}{(\zeta^2 - 1)^k (\xi^2 - 1)^l} = 0,$$

which means that

$$[\mathbf{c}_k, \mathbf{c}_l]_+ = 0, \quad k, l \geq 0. \quad (3.18)$$

The same structure applies to all commutation relations, except for $[\mathbf{b}^*(\zeta), \mathbf{b}(\xi)]_+$ and $[\mathbf{c}^*(\zeta), \mathbf{c}(\xi)]_+$. These relations are the reason for introducing the additional factor ζ^2 in the expansions of the fermionic creation

operators. Using the known expansions for $\mathbf{x}^* = \mathbf{b}^*, \mathbf{c}^*$ and a corresponding $\mathbf{x} = \mathbf{b}, \mathbf{c}$ we can write

$$\begin{aligned} [\mathbf{x}^*(\zeta), \mathbf{x}(\xi)]_+ &= (\zeta/\xi)^{\alpha s(\mathbf{x}^*)} \zeta^2 \sum_{\substack{p=1 \\ k=0}}^{\infty} \frac{(\zeta^2 - 1)^{p-1}}{(\xi^2 - 1)^k} [\mathbf{x}_p^*, \mathbf{x}_k]_+ \\ &= -\psi(\zeta/\xi, \alpha s(\mathbf{x}^*)) = \frac{1}{2} \frac{\xi^2 + \zeta^2}{\xi^2 - \zeta^2} (\zeta/\xi)^{\alpha s(\mathbf{x}^*)} . \end{aligned} \quad (3.19)$$

And with the already known expansion (2.49) we then obtain

$$\begin{aligned} &\sum_{\substack{p=1 \\ k=0}}^{\infty} \frac{(\zeta^2 - 1)^{p-1}}{(\xi^2 - 1)^k} [\mathbf{x}_p^*, \mathbf{x}_k]_+ \\ &= \sum_{p=1}^{\infty} (\zeta^2 - 1)^{p-1} [\mathbf{x}_p^*, \mathbf{x}_0]_+ + \sum_{\substack{p=1 \\ k=1}}^{\infty} \frac{(\zeta^2 - 1)^{p-1}}{(\xi^2 - 1)^k} [\mathbf{x}_p^*, \mathbf{x}_k]_+ \\ &= \frac{1}{2} \sum_{k=0}^{\infty} (-1)^k (\zeta^2 - 1)^k + \frac{1}{\xi^2 - 1} \sum_{k=0}^{\infty} \left(\frac{\zeta^2 - 1}{\xi^2 - 1} \right)^k . \end{aligned} \quad (3.20)$$

This gives us

$$[\mathbf{x}_p^*, \mathbf{x}_0]_+ = \frac{1}{2} (-1)^{p-1} , \quad [\mathbf{x}_p^*, \mathbf{x}_k]_+ = \delta_{p,k} , \quad (3.21)$$

which is consistent with the definition of the modes \mathbf{x}_0 (2.54), (2.71). At this point it is also clear that the coefficients $\tilde{\mathbf{x}}_p^* = \mathbf{x}_p^* + \mathbf{x}_{p-1}^*$ would not satisfy fermionic anticommutation relations.

With that, the commutation relations of the modes for $p, k \geq 1$ are

$$[\mathbf{t}_p^*, \mathbf{x}_k] = 0 , \quad (3.22)$$

where $\mathbf{x} = \mathbf{t}^*, \mathbf{b}^*, \mathbf{c}^*, \mathbf{b}, \mathbf{c}$. And

$$[\mathbf{b}_p, \mathbf{b}_k]_+ = [\mathbf{b}_p, \mathbf{c}_k]_+ = [\mathbf{c}_p, \mathbf{c}_k]_+ = 0 , \quad (3.23a)$$

$$[\mathbf{b}_p^*, \mathbf{b}_k^*]_+ = [\mathbf{b}_p^*, \mathbf{c}_k^*]_+ = [\mathbf{c}_p^*, \mathbf{c}_k^*]_+ = 0 , \quad (3.23b)$$

$$[\mathbf{b}_p^*, \mathbf{c}_k]_+ = [\mathbf{c}_p^*, \mathbf{b}_k]_+ = 0 , \quad (3.23c)$$

$$[\mathbf{b}_p^*, \mathbf{b}_k]_+ = [\mathbf{c}_p^*, \mathbf{c}_k]_+ = \delta_{p,k} . \quad (3.23d)$$

3.2 Fermionic Basis

In this section we will show that the creation operators define a basis of the space $\mathcal{W}^{(\alpha)}$ and how to construct a basis of the space $\mathcal{W}_{[1,n]}^{(\alpha)}$ using modes of

the creation operators. Following reference [51], the interval $[1, n]$ is chosen, which can be done because of translational invariance. In [51] it is shown how to choose elements from the family

$$(\mathbf{t}_1^*)^p \mathbf{t}_{i_1}^* \cdots \mathbf{t}_{i_r}^* \mathbf{b}_{j_1}^* \cdots \mathbf{b}_{j_s}^* \mathbf{c}_{k_1}^* \cdots \mathbf{c}_{k_t}^* (q^{2\alpha S(0)}) , \quad (3.24)$$

$$i_1 \geq \cdots \geq i_r \geq 2, \quad j_1 > \cdots > j_s \geq 1, \quad k_1 > \cdots > k_t \geq 1, \quad p \in \mathbb{Z}, \quad r, s, t \geq 0$$

in such a way that they form a basis of $\mathcal{W}_{[1,n]}^{(\alpha)}$.

3.2.1 Linear Independence

To show that the elements (3.24) form a basis we first need to establish that they are linearly independent. Without the modes \mathbf{t}_i^* (i.e. for $p = r = 0$ in 3.24) this would be clear because they would be created by regular fermions only. The operators \mathbf{t}_p^* lack corresponding annihilation operators however, so we can not assume that they are regular bosons. Because of this, special care has to be taken when showing that (3.24) are linearly independent. To address this issue an operator

$$\mathbf{h}^*(\zeta) = (\mathbf{t}_1^*)^{-1} \mathbf{t}^*(\zeta) = \sum_{p=0}^{\infty} (\zeta^2 - 1)^p \mathbf{h}_p^* \quad (3.25)$$

is introduced, where obviously

$$\mathbf{h}_p^* = (\mathbf{t}_1^*)^{-1} \mathbf{t}_{p+1}^* . \quad (3.26)$$

Note that $\tau = \mathbf{t}_1^*/2$ is the shift by one lattice site to the right.

Then lemma 2.1 of [51] shows that the set of elements

$$(\mathbf{h}_1^*)^{m_1} (\mathbf{h}_2^*)^{m_2} \cdots (q^{2\alpha S(0)}) , \quad m_1, m_2, \cdots \geq 0 \quad (3.27)$$

is linearly independent. In the proof of this lemma it is shown that the operator $\mathbf{h}^*(\zeta)$ can be expressed as

$$\mathbf{h}^*(\zeta) = (1 - z^2) \exp \left(\sum_{\nu=1}^{\infty} \frac{z^\nu}{\nu} (I_{-\nu} - I_\nu) \right) \quad (3.28)$$

where

$$z = \frac{1 - \zeta^2}{1 + \zeta^2} \quad (3.29)$$

and with bosonic operators I_ν that satisfy

$$[I_\mu, I_\nu] = 2\mu\delta_{\mu+\nu,0} , \quad (3.30)$$

$$I_\nu(q^{2\alpha S(0)}) = 0 \quad \text{for } \nu > 0 . \quad (3.31)$$

We feel that the last step in the proof, i.e. concluding linear independence from (3.28), needs further explanation.

First we show that the modes of $\ln \mathbf{h}^*(\zeta)$ are linearly independent. Using the Taylor expansion of the logarithm we write

$$\ln \mathbf{h}^*(\zeta) = \sum_{\nu=1}^{\infty} \frac{z^\nu}{\nu} (I_{-\nu} - I_\nu - (1 - (-1)^{\nu-1})) =: \sum_{\nu=1}^{\infty} \frac{z^\nu}{\nu} \mathbb{I}_\nu \quad (3.32)$$

Since the I_ν are linearly independent, the operators \mathbb{I}_ν have to be independent as well. We now write $\ln \mathbf{h}^*(\zeta)$ as an expansion in ζ^2 around $\zeta^2 = 1$. Using

$$\frac{1}{1 + \zeta^2} = \sum_{k=0}^{\infty} \frac{(1 - \zeta^2)^k}{2^{k+1}}$$

we get

$$\ln \mathbf{h}^*(\zeta) = \sum_{\nu=1}^{\infty} \left[\sum_{k=1}^{\infty} \frac{(-1)^k}{2^k} (\zeta^2 - 1)^k \right]^\nu \frac{\mathbb{I}_\nu}{\nu} =: \sum_{\nu=1}^{\infty} (\zeta^2 - 1)^\nu \boldsymbol{\eta}_\nu^* . \quad (3.33)$$

It follows that

$$\boldsymbol{\eta}_p^* = \mathcal{O}(\mathbb{I}_p) , \quad (3.34)$$

where the order $\mathcal{O}(\mathbb{I}_p)$ means that \mathbb{I}_p is the operator with the highest index. Because of this trigonal shape the coefficients $\boldsymbol{\eta}_p^*$ of $\ln \mathbf{h}^*(\zeta)$ are linearly independent.

From this we can conclude that the coefficients of $\mathbf{h}^*(\zeta)$ are independent as well. To do this we give an alternative form of the expansion of $\ln \mathbf{h}^*(\zeta)$ using (3.25). Knowing that $\mathbf{h}_0^* = 1$, we can write

$$\ln \mathbf{h}^*(\zeta) = - \sum_{\nu=1}^{\infty} \frac{1}{\nu} \left[- \sum_{p=1}^{\infty} (\zeta^2 - 1)^p \mathbf{h}_p^* \right]^\nu . \quad (3.35)$$

Again, we can observe a trigonal shape:

$$\boldsymbol{\eta}_p^* = \mathcal{O}(\mathbf{h}_p^*) . \quad (3.36)$$

Since no diagonal element is equal to zero, this is invertible:

$$\mathbf{h}_p^* = \mathcal{O}(\boldsymbol{\eta}_p^*) . \quad (3.37)$$

From this it follows that the coefficients of $\mathbf{h}^*(\zeta)$ are linearly independent, meaning that the elements (3.27) are independent.

Since the \mathbf{t}_p^* commute with all other operators (3.22), it is clear that the elements (3.24) are linearly independent as mentioned above.

3.2.2 Support Property

The support of the elements (3.24) themselves is unknown in general. In order to construct a basis of $\mathcal{W}_{[1,n]}^{(\alpha)}$, elements have to be chosen which are supported on the interval $[1, n]$. To achieve this, a family of operators B_J is introduced, indexed by $J \subset [1, n]$. Writing $l = |J|$ they are defined by

$$B_J = \sum_{I,K} C_{J,K}^I \mathbf{b}_n^* \cdots \mathbf{c}_{k_1}^{i_1} \cdots \mathbf{c}_{k_l}^{i_l} \cdots \mathbf{b}_1^*(q^{2\alpha S(0)}) . \quad (3.38)$$

The sum is taken over all subsets $I, K \subset [1, n]$ with $I = \{i_1, \dots, i_l\}$ and $K = \{k_1, \dots, k_l\}$. The operators $\mathbf{c}_{k_p}^*$ are placed at the i_p -th slot counting from the right, replacing the corresponding operator $\mathbf{b}_{i_p}^*$. It is then shown in section 3.1 of [51] that the support of these operators is contained in $[1, n]$ for a suitable choice of the coefficients $C_{J,K}^I$.

For this proof the aforementioned ‘‘barred’’ operators $\bar{\mathbf{c}}(\zeta)$, $\bar{\mathbf{b}}(\zeta)$, $\bar{\mathbf{c}}^*(\zeta)$, $\bar{\mathbf{b}}^*(\zeta)$ are used. Since they appear only in this chapter, we will not discuss them at length. The crucial point in the context of this proof is their support property. The annihilation operators do not change the support, whereas the creation operators enlarge the support essentially to the left. For $X \in (\mathcal{W}^{(\alpha)})_{[k,l]}$ we have

$$\text{supp } \bar{\mathbf{x}}_p^*(X) \subset [k - p + 1, l + 1] , \quad (\bar{\mathbf{x}}^* = \bar{\mathbf{b}}^*, \bar{\mathbf{c}}^*) . \quad (3.39)$$

The coefficients $C_{J,K}^I$ are now chosen in such a way that

$$B_J = \sum_{I,K} C_{J,K}^I \bar{\mathbf{b}}_n^* \cdots \bar{\mathbf{c}}_{k_1}^{i_1} \cdots \bar{\mathbf{c}}_{k_l}^{i_l} \cdots \bar{\mathbf{b}}_1^*(q^{2\alpha S(0)}) . \quad (3.40)$$

If this is true, obviously we have

$$\text{supp } B_J \subset [1, \infty) \cap (-\infty, n] = [1, n] . \quad (3.41)$$

The above statement is true, if the $C_{J,K}^I$ obey the equation

$$\frac{\Delta(x)\Delta(y)\Delta(z)}{\prod_{i,j=1}^l (1 - x_i y_j)(1 - x_i z_j)} = \sum C_{j_1, \dots, j_l; k_1, \dots, k_l}^{i_1, \dots, i_l} \prod_{p=1}^l (x_p^{i_p-1} y_p^{j_p-1} z_p^{k_p-1}) . \quad (3.42)$$

Here $x = (x_1, \dots, x_l)$, $y = (y_1, \dots, y_l)$, $z = (z_1, \dots, z_l)$ and $\Delta(x) = \prod_{1 \leq i < j \leq l} (x_i - x_j)$. The sum is taken over all positive integers i_p, j_p, k_p ($p = 1, \dots, l$). Decreasing series ($i_1 > \dots > i_l$, etc.) are identified with subsets $I = \{i_1, \dots, i_l\} \subset [1, n]$, etc. It can then be shown that the coefficients $C_{J,K}^I$ coincide with the Littlewood-Richardson coefficients $c_{\mu, \nu}^\lambda$ (see [56]). The exact correspondence is

$$C_{J,K}^I = c_{\lambda(J), \lambda(K)}^{\lambda(I)} \quad (3.43)$$

with $\lambda(I) = (\lambda_1, \dots, \lambda_l) = (i_1 - l, \dots, i_l - 1)$.

Now we can show the linear independence of the B_J , using the fact that $c_{\mu, \emptyset}^\lambda = \delta_{\lambda, \mu}$. Using the mapping above, it is clear that $\lambda(K) = \emptyset$ for $K = \{l, \dots, 1\}$. Then we get

$$B_J = \pm \mathbf{b}_{\bar{J}}^* \mathbf{c}_{\{1, \dots, l\}}^* (q^{2\alpha S(0)}) + \dots \quad (3.44)$$

where no term in “...” contains the group $\mathbf{c}_{\{1, \dots, l\}}^*$ and \bar{J} is the complement of J with respect to $[1, n]$. From this it follows directly, that the B_J have to be linearly independent.

3.2.3 Littlewood-Richardson Rule

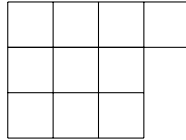
The explicit form of the elements B_J is later needed to construct the fermionic basis. To be able to calculate this form, one has to calculate the Littlewood-Richardson coefficients $c_{\mu, \nu}^\lambda$. We did this by using the Littlewood-Richardson rule as explained in [56]. Here we want to give just a brief overview of the necessary definitions to be able to formulate the Littlewood-Richardson rule.

Let us first define a partition to be a sequence

$$\lambda = (\lambda_1, \lambda_2, \dots) \quad (3.45)$$

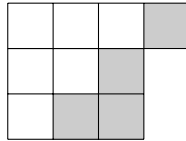
of non-negative integers in decreasing order ($\lambda_1 \geq \lambda_2 \geq \dots$). The length of λ , denoted by $\ell(\lambda)$ is the number of its non-zero entries. The weight of λ is the sum of its parts: $|\lambda| = \lambda_1 + \lambda_2 + \dots$.

The diagram of a partition λ is the set of points $(i, j) \in \mathbb{Z}^2$ such that $1 \leq j \leq \lambda_i$. Normally the points are represented as squares. For drawing diagrams, we use the same convention as for matrices, where the first coordinate i is the row index and the second coordinate j is the column index. For example the diagram of the partition $\lambda = (433)$ would be



The conjugate of the partition λ is the partition λ' whose diagram is the transpose of the diagram of λ . For the example above, we would have $\lambda' = (3331)$.

For two partitions λ, μ we write $\lambda \supset \mu$ if the diagram of λ contains the diagram of μ , i.e. $\lambda_i \geq \mu_i$ for all $i \geq 1$. Then the difference $\theta = \lambda - \mu$ is called a skew diagram. For example, if $\lambda = (433)$ and $\mu = (321)$, the skew diagram $\lambda - \mu$ is the shaded region in



A skew diagram θ is called a horizontal strip if it has at most one square in each column, i.e. $\theta'_i \leq 1$.

A tableau T is then a sequence of partitions

$$\lambda = \lambda^{(r)} \supset \dots \supset \lambda^{(1)} \supset \lambda^{(0)} = \mu \quad (3.46)$$

such that each skew diagram $\theta^{(i)} = \lambda^{(i)} - \lambda^{(i-1)}$ for $1 \leq i \leq r$ is a horizontal strip. Graphically this is represented by numbering each square of the skew diagram $\theta^{(i)}$ with the number i . For example say that $\lambda^{(2)} = (433)$, $\lambda^{(1)} = (332)$ and $\lambda^{(0)} = (321)$. Then T would be

$$\begin{array}{c} \boxed{2} \\ \boxed{1} \\ \boxed{1} \quad \boxed{2} \end{array}$$

It is then clear, that the numbers must increase strictly down each column and weakly from left to right along a row. The skew diagram $\lambda - \mu$ is called the shape of T and the sequence $(|\theta^{(1)}|, \dots, |\theta^{(r)}|)$ is called the weight of T .

Lastly, the word of a tableau T is the sequence $w(T)$ derived by reading the numbers in T from right to left and top to bottom. In our example this is $w(T) = (2121)$. A word $w = a_1 \dots a_N$ in the symbols $1, \dots, n$ is called a lattice permutation if for $1 \leq r \leq N$ and $1 \leq i < n$, the number of occurrences of the symbol i in $a_1 \dots a_r$ is not less than the number of occurrences of $i + 1$.

We can now formulate the Littlewood-Richardson rule:

Let λ, μ, ν be partitions. Then $c_{\mu, \nu}^{\lambda}$ is equal to the number of tableaux T of shape $\lambda - \mu$ and weight ν such that $w(T)$ is a lattice permutation.

3.2.4 Basis of $(\mathcal{W}^{(\alpha)})_{[1, n]}$

With the B_J we now have a set of operators whose support is contained in $[1, n]$. To construct a basis we apply annihilation operators on the B_J . Since the annihilation operators preserve the support, the resulting operators will also be contained in $[1, n]$. For a subset $I = \{i_1, \dots, i_l\} \subset [1, n]$ ($i_1 > \dots > i_l$) we write

$$\mathbf{x}_I = \mathbf{x}_{i_1} \cdots \mathbf{x}_{i_l} . \quad (3.47)$$

In section 3.2 of [51] it is then proven, that the elements

$$\bar{\mathbf{b}}_M \mathbf{c}_N (B_J) \quad (J \subset [1, n], M \subset [1, n - |J|], N \subset [1, |J|]) \quad (3.48)$$

form a basis of $(\mathcal{W}^{(\alpha)})_{[1, n]}$. Since there is a total of 4^n possible choices for J, M, N and the support of these elements is contained in $[1, n]$, it only remains to show, that they are linearly independent. To prove this, we need the anticommutation relations

$$[\mathbf{b}_p^*, \bar{\mathbf{b}}_{p'}]_+ = -\mathbf{t}_{p-p'+1}^* , \quad [\bar{\mathbf{b}}_p, \mathbf{c}_{p'}]_+ = 0 \quad (3.49)$$

which are proven in [50].

Since not every detail of the proof of theorem 3.3 in [51] may be obvious to the reader, we will provide some additional details and a slight variation to the original proof. The authors start with a combination

$$\sum_{M,N,J} A_{M,N,J} \bar{\mathbf{b}}_M \mathbf{c}_N(B_J) = 0 \quad (3.50)$$

where the sum is taken over $J \subset [1, n]$, $M \subset [1, n-l]$, $N \subset [1, l]$, $l = |J|$. Since every term contains $n-l$ number of \mathbf{b}^* and \mathbf{t}^* , this sum has to be separately zero for each l . Now choose $M_0 \subset [1, n-l]$, $N_0 \subset [1, l]$ and multiply by $\bar{\mathbf{b}}_{[1, n-l] \setminus M_0} \mathbf{c}_{[1, l] \setminus N_0}$. After applying this factor, the only terms remaining in (3.50) will be the ones for which $M \subset M_0$ and $N \subset N_0$. Every other term will contain a squared annihilation operator. It can then be shown recursively that all coefficients $A_{M,N,J}$ have to be zero.

Starting with $M_0 = N_0 = \emptyset$, we obtain

$$\sum_{|J|=l} A_{\emptyset, \emptyset, J} \bar{\mathbf{b}}_{[1, n-l]} \mathbf{c}_{[1, l]}(B_J) = 0. \quad (3.51)$$

We know from (3.44) that B_J contains only one term with the group $\mathbf{c}_{[1, l]}^*$, which is the only term that does not vanish. Using this, we obtain

$$\sum_{|J|=l} (\pm)_J A_{\emptyset, \emptyset, J} \bar{\mathbf{b}}_{[1, n-l]} \mathbf{b}_J^*(q^{2\alpha S(0)}) = 0 \quad (3.52)$$

where $(\pm)_J$ signifies some sign which depends on J . This can then be represented using a determinant and $\bar{J} = \{j'_1, \dots, j'_{n-l}\}$ as

$$\begin{aligned} & \sum_{|J|=l} (\pm)_J A_{\emptyset, \emptyset, J} \det \left(\mathbf{t}_{j'_a - b + 1}^* \right)_{1 \leq a, b \leq n-l} (q^{2\alpha S(0)}) \\ &= (\mathbf{t}_1^*)^{n-l} \sum_{|J|=l} (\pm)_J A_{\emptyset, \emptyset, J} \det \left(\mathbf{h}_{j'_a - b}^* \right)_{1 \leq a, b \leq n-l} (q^{2\alpha S(0)}) \\ &= 0. \end{aligned} \quad (3.53)$$

The last step is true because $\mathbf{t}_1^*/2$ is a shift by one place to the right and therefore invertible. Since it was already proven that monomials in \mathbf{h}_p^* are linearly independent, we know from the theory of symmetric functions that the polynomials induced by the determinants must be independent as well. From this it follows that

$$A_{\emptyset, \emptyset, J} = 0 \quad \text{for } J \subset [1, n]. \quad (3.54)$$

Using the same construction one can now recursively show that all other coefficients have to be zero as well. If we choose $M_0 = \emptyset$ and $N_0 = \{n_1\}$ we can show that $A_{\emptyset, \{n_1\}, J} = 0$ by using the now known coefficients $A_{\emptyset, \emptyset, J}$.

It then follows that all $A_{M,N,J}$ have to be zero. Thus the elements from (3.48) have to be linearly independent and form a basis of $(\mathcal{W}^{(\alpha)})_{[1, n]}$.

Chapter 4

Expectation Values

In this chapter we will explain how to calculate correlation functions for the XXZ model. This will be achieved using two different techniques: on the one hand we will use a theorem [52] by Jimbo, Miwa and Smirnov and on the other hand we will use the exponential form of the density matrix as explained in [53].

4.1 JMS Theorem

The JMS theorem proven in [52] explains how to calculate the expectation value of an operator constructed by applying a set of creation operators on the vacuum:

$$\mathbf{t}^*(\zeta_1^0) \cdots \mathbf{t}^*(\zeta_k^0) \mathbf{b}^*(\zeta_1^+) \cdots \mathbf{b}^*(\zeta_l^+) \mathbf{c}^*(\zeta_l^-) \cdots \mathbf{c}^*(\zeta_1^-) (q^{2\alpha S(0)}) .$$

Using this theorem, we will show how to calculate expectation values of operators, constructed by modes of creation operators instead of their generating functions. This is done in order to easily calculate expectation values of the elements of the fermionic basis. It is then possible to cover arbitrary operators by expressing them in terms of the fermionic basis.

Before we can use the theorem, we need to explain how an expectation value is defined in the context of [52]. In [49, 50] the authors considered vacuum expectation values of local operators \mathcal{O} :

$$\langle q^{2\alpha S(0)} \mathcal{O} \rangle = \frac{\langle \text{vac} | q^{2\alpha S(0)} \mathcal{O} | \text{vac} \rangle}{\langle \text{vac} | q^{2\alpha S(0)} | \text{vac} \rangle} . \quad (4.1)$$

This is only a formal expression, because the ground state $|\text{vac}\rangle$ is not defined on an infinite chain. Zero-temperature expectation values for the infinite chain are defined in a proper manner in [47] for the XXX model and in [48] for the XXZ model. In these works the reduced density matrix is obtained as a solution of the reduced quantum Knizhnik-Zamolodchikov equation. This

was later generalized by Boos, Göhmann, Klümper and Suzuki in [57] to the case of a finite temperature and non-zero magnetic field:

$$\langle q^{2\alpha S(0)} \mathcal{O} \rangle_{T,h} = \text{tr}_{1,\dots,n} \left(D_n(T, h) q^{2\alpha S(0)} \mathcal{O} \right) \quad (4.2)$$

where $D_n(T, h)$ is the reduced density matrix for an interval of length n on an infinite chain. The authors use a multiple integral representation of the density matrix to derive a representation in terms of exponentials of fermionic annihilation operators. Interestingly, this means that the fermionic structure is not a special property of vacuum expectation values but is instead more deeply tied to the model.

In [52] a generalization to the thermal expectation value is introduced. The authors define a Matsubara space (named Trotter space by other authors)

$$\mathcal{H}_M = \mathbb{C}^{2s_1+1} \otimes \dots \otimes \mathbb{C}^{2s_n+1} , \quad (4.3)$$

where s_m is an arbitrary spin and an inhomogeneity τ_m is attached to each component. Then the expectation value is

$$Z^\kappa \left\{ q^{2\alpha S(0)} \mathcal{O} \right\} = \lim_{l \rightarrow \infty} \frac{\text{tr}_M \text{tr}_{[-l+1,l]} \left(T_{[-l+1,l],M} q^{2\kappa S_{[-l+1,l]} + 2\alpha S_{[-l+1,0]}} \mathcal{O} \right)}{\text{tr}_M \text{tr}_{[-l+1,l]} \left(T_{[-l+1,l],M} q^{2\kappa S_{[-l+1,l]} + 2\alpha S_{[-l+1,0]}} \right)} , \quad (4.4)$$

where tr_M is the trace over \mathcal{H}_M . In the context of [52] a missing argument implies it to be one, e.g. $T_{[-l+1,l],M} = T_{[-l+1,l],M}(1)$. This definition is then simplified to be

$$Z^\kappa \left\{ q^{2\alpha S(k-1)} X_{[k,m]} \right\} = \rho(1)^{k-1} \frac{\langle \kappa + \alpha | \text{tr}_{[k,m]} (T_{[k,m],M} q^{2\kappa S_{[k,m]}} X_{[k,m]}) | \kappa \rangle}{\Lambda(1, \kappa)^{m-k+1} \langle \kappa + \alpha | \kappa \rangle} \quad (4.5)$$

where $|\kappa\rangle$ is an eigenvector of the vertical transfer matrix $T_M(1, \kappa)$ and $\langle \kappa + \alpha |$ an eigenvector of $T_M(1, \kappa + \alpha)$. $\Lambda(1, \kappa)$ is then the eigenvalue of $T_M(1, \kappa)$ corresponding to $|\kappa\rangle$. These vectors have to satisfy the condition

$$\langle \kappa + \alpha | \kappa \rangle \neq 0 . \quad (4.6)$$

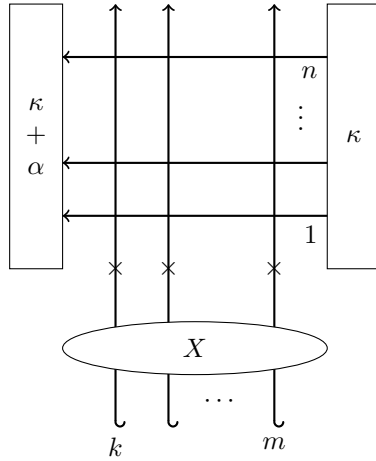
The function ρ is defined as the ratio of the two eigenvalues corresponding to the vectors chosen:

$$\rho(\zeta) = \frac{\Lambda(\zeta, \kappa + \alpha)}{\Lambda(\zeta, \kappa)} . \quad (4.7)$$

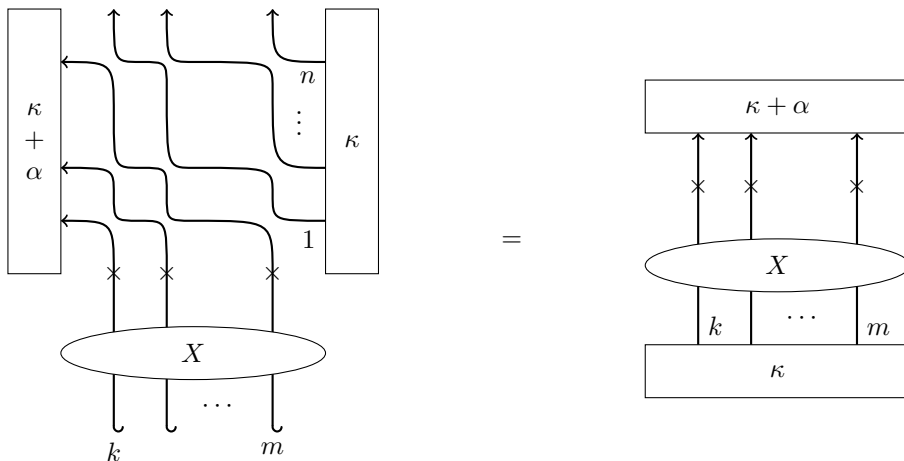
The fact that apparently two expressions are used for the generalized expectation value may be a source of confusion. In [52] the authors start with the expression (4.4) and then show that it simplifies to (4.5) if $\langle \kappa + \alpha |$ and $|\kappa\rangle$ are eigenvectors corresponding to the eigenvalues of largest modulus. But then the expression (4.5) is used as the definition of the generalized expectation value for arbitrary eigenvectors of the vertical transfer matrix which only have to obey (4.6).

It is then possible to calculate expectation values for different density matrices by choosing appropriate values for s_m and τ_m . This is demonstrated in [58]. Since the two examples given in this paper are the ones most relevant to us, we shall shortly explain them.

One example for such a choice is the case of zero temperature and finite length. This can be obtained by choosing $s_m = \frac{1}{2}$ and $\tau_m = 1$ for $m = 1, \dots, n$ where n will be the length of the resulting system. Note that in [58] another choice for τ_m is made, in order to obtain simpler integration paths for the auxiliary functions. To make such a choice one has to change the definition (4.4) where the spectral parameter is set to $\zeta = 1$. The important point is to choose the spectral parameter and the inhomogeneities so that the R matrices become permutation operators, $R_{12}(0) = P_{12}$. It is easy to understand graphically, what happens for the above-mentioned choice of parameters. The numerator in (4.5) is represented graphically as



If we choose $n = \ell(X_{[k,m]}) = m - k + 1$ and $\tau_m = 1$ this becomes



Now it is clear that the functional Z^κ becomes a matrix element for the two states $\langle \kappa + \alpha |$ and $|\kappa \rangle$ on a chain of length n . These two states can be chosen

freely, as long as they satisfy the condition (4.6). The choice of these states will then fix the functions ρ and ω .

The second example given in [58] is that of thermal expectation values for an infinite chain. These can be obtained by setting $\beta_{2j-1} = \eta - \frac{\beta}{N}$ and $\beta_{2j} = \frac{\beta}{N}$ for $j = 1, \dots, N/2$. Here the β_m are the additive inhomogeneities corresponding to the τ_m : $\tau_m = e^{\beta_m}$. The crossing symmetry and unitarity of the R matrix then yields the desired expectation values.

In [52] a set of relations regarding the generalized expectation values is derived:

$$Z^\kappa \{ \mathbf{t}^*(\zeta)(X) \} = 2\rho(\zeta) Z^\kappa \{ X \} , \quad (4.8)$$

$$Z^\kappa \{ \mathbf{b}^*(\zeta)(X) \} = \frac{1}{2\pi i} \oint_\Gamma \frac{d\xi^2}{\xi^2} \omega(\zeta, \xi) Z^\kappa \{ \mathbf{c}(\xi)(X) \} , \quad (4.9)$$

$$Z^\kappa \{ \mathbf{c}^*(\zeta)(X) \} = -\frac{1}{2\pi i} \oint_\Gamma \frac{d\xi^2}{\xi^2} \omega(\zeta, \xi) Z^\kappa \{ \mathbf{b}(\xi)(X) \} . \quad (4.10)$$

The paper considers the homogeneous case, therefore Γ encircles $\xi^2 = 1$. From these relations follow the definitions for the functions ρ and ω :

$$\rho(\zeta) = \frac{1}{2} Z^\kappa \left\{ \mathbf{t}^*(\zeta)(q^{2\alpha S(0)}) \right\} , \quad (4.11)$$

$$\omega(\zeta, \xi) = Z^\kappa \left\{ \mathbf{b}^*(\zeta) \mathbf{c}^*(\xi)(q^{2\alpha S(0)}) \right\} . \quad (4.12)$$

The main result of the paper also follows directly from these relations:

$$\begin{aligned} Z^\kappa \left\{ \mathbf{t}^*(\zeta_1^0) \cdots \mathbf{t}^*(\zeta_k^0) \mathbf{b}^*(\zeta_1^+) \cdots \mathbf{b}^*(\zeta_l^+) \mathbf{c}^*(\zeta_l^-) \cdots \mathbf{c}^*(\zeta_1^-)(q^{2\alpha S(0)}) \right\} \\ = \prod_{p=1}^k 2\rho(\zeta_p^0) \times \det \left(\omega(\zeta_i^+, \zeta_j^-) \right)_{i,j=1,\dots,l} . \end{aligned} \quad (4.13)$$

The choice of the parameters s_m and τ_m is completely absorbed in the two functions $\rho(\zeta)$ and $\omega(\zeta, \xi)$. We can now use (4.13) to compute expectation values for elements of the fermionic basis in terms of the two functions $\rho(\zeta)$ and $\omega(\zeta, \xi)$. To obtain the according thermal expectation value (4.2) we then need to choose two appropriate functions which are derived in [58].

Before we consider the correct choice of functions, we will derive an expression for the generalized expectation values when using the modes of the fermionic creation operators. On the left-hand side we insert the Taylor expansions for the creation operators and on the right-hand side we can do

an expansion in all parameters. By comparison of coefficients we then obtain

$$Z^\kappa \left\{ \mathbf{t}_{p_1}^* \cdots \mathbf{t}_{p_k}^* \mathbf{b}_{r_1}^* \cdots \mathbf{b}_{r_l}^* \mathbf{c}_{s_1}^* \cdots \mathbf{c}_{s_l}^* (q^{2\alpha S(0)}) \right\} =$$

$$2^k \prod_{i=1}^k \frac{\partial^{p_i-1}}{(\zeta_i^0)^2} \rho(\zeta_i^0) \Big|_{(\zeta_i^0)^2=1} \left[\prod_{i=1}^l \frac{\partial^{r_i-1}}{(\zeta_i^+)^2} \frac{\partial^{s_i-1}}{(\zeta_i^-)^2} \left(\frac{\zeta_i^-}{\zeta_i^+} \right)^\alpha (\zeta_i^+ \zeta_i^-)^{-2} \right]$$

$$\det \left(\omega(\zeta_i^+, \zeta_j^-) \right)_{i,j=1,\dots,l} \Big|_{(\zeta_i^+)^2=(\zeta_i^-)^2=1} . \quad (4.14)$$

Note that the functions ρ and ω are defined differently in various works. Up until now we used the definitions given in [52]. Let us first consider the function $\rho(\zeta)$. In [58] it is defined in the same way as in [52]. In [53] however a slightly different function is used, namely the function $\tilde{\rho}(\lambda)$ which depends on the additive spectral parameter $\lambda = \ln \zeta$. The function $\rho(\zeta)$ itself will not enter the end result. Instead, a function $\varphi(\lambda, \alpha)$ will be used which is introduced in [57]. The relation between ρ and φ can be seen using the formula

$$\varphi(\lambda, 0) = -2T \frac{\partial}{\partial h} \ln \Lambda(\lambda) \quad (4.15)$$

from [57] (note that there is a mistake in this paper, as the factor -2 is missing), where $\Lambda(\lambda)$ is the largest eigenvalue of the quantum transfer matrix. From this it follows that φ is related to the magnetization through

$$\varphi(0, 0) = -2m(T, h) . \quad (4.16)$$

With the definition of ρ ,

$$\rho(\zeta) = \frac{\Lambda(\zeta, \alpha + \kappa)}{\Lambda(\zeta, \kappa)} \quad (4.17)$$

from [52] (where the eigenvalues are named T) and the relation

$$\kappa = \frac{h}{2\eta T} \quad (4.18)$$

from [58] we obtain

$$\partial_\alpha \rho(\zeta, \alpha) \Big|_{\alpha=0} = \partial_\kappa \ln \Lambda(\zeta, \kappa) = 2\eta T \partial_h \ln \Lambda(\zeta, \kappa) . \quad (4.19)$$

It follows that

$$\partial_\alpha \rho(\zeta, \alpha) \Big|_{\alpha=0} = -\eta \varphi(\lambda, 0) . \quad (4.20)$$

Note that this is not consistent with [58], where the sign of α was changed. This can be seen by comparing equation (12) in [57] to equation (32) in [58]. This is consistent with

$$\rho(1) = 1 + 2\eta \alpha m(T, h) + \mathcal{O}(\alpha^2) \quad (4.21)$$

from [58].

Let us now discuss the function ω . The function used up until now is defined in [52]. In [53, 57] another function is used, which is also called ω in these papers. We will denote it by $\tilde{\omega}$. It is shown in [58] that $\tilde{\omega}(\mu_1, \mu_2; \alpha) = -\omega(\zeta_1, \zeta_2; \alpha) + \omega_0(\zeta_1/\zeta_2; \alpha)$ in the limit $\alpha \rightarrow 0$, for a certain function ω_0 introduced in [50]. Since existing programs calculate the function $\tilde{\omega}(\mu_1, \mu_2) = e^{\alpha(\mu_2 - \mu_1)} \tilde{\omega}(\mu_1, \mu_2)$, we will express the expectation values in terms of this function. It is important to note that $\zeta^{-\alpha} \omega_0(\zeta, \alpha) = \mathcal{O}(\alpha^2)$, which allows us to just replace ω by $\tilde{\omega}$ in the limit $\alpha \rightarrow 0$, since $(\zeta_1/\zeta_2)^{-\alpha} \omega(\zeta_1, \zeta_2; \alpha) = \mathcal{O}(\alpha)$. The reason for introducing ω_0 at all is that it is used in [50] to calculate vacuum expectation values for the fermionic basis. In this work however, it is not important. We can then write

$$Z^\kappa \left\{ \mathbf{t}_{p_1}^* \cdots \mathbf{t}_{p_k}^* \mathbf{b}_{r_1}^* \cdots \mathbf{b}_{r_l}^* \mathbf{c}_{s_1}^* \cdots \mathbf{c}_{s_l}^* (q^{2\alpha S(0)}) \right\}_{\alpha \rightarrow 0} = 2^k \prod_{i=1}^k \frac{\partial_{\zeta_i^2}^{p_i-1} \rho(\ln \zeta_i)}{(p_i-1)!} \Bigg|_{\zeta_i^2=1} \\ \times (-1)^l \det \left(\frac{\partial_{(\zeta_i^+)^2}^{r_i-1}}{(r_i-1)!} \frac{\partial_{(\zeta_j^-)^2}^{s_j-1}}{(s_j-1)!} \frac{\tilde{\omega}(\ln \zeta_i^+, \ln \zeta_j^-)}{(\zeta_i^+ \zeta_j^-)^2} \right) \Bigg|_{(\zeta_i^+)^2 = (\zeta_i^-)^2 = 1} \Bigg|_{i,j=1,\dots,l} . \quad (4.22)$$

To calculate multiple derivatives on the computer we then derived the formula

$$\partial_{\zeta^2}^n \frac{f(\ln \zeta)}{\zeta^{2m}} = \sum_{k=0}^{\infty} B_m(n, k) \frac{f^{(k)}(\ln \zeta)}{\zeta^{2(n+m)}} , \quad (4.23a)$$

where

$$B_m(0, 0) = 1 , \quad (4.23b)$$

$$B_m(n, k) = 0 \quad \text{if } k < 0 \text{ or } k > n , \quad (4.23c)$$

$$B_m(n, k) = \frac{1}{2} B_m(n-1, k-1) - (n+m-1) B_m(n-1, k) \quad \text{else.} \quad (4.23d)$$

Using this it will become easy to compare to the results of [53] where correlation functions are given in terms of derivatives of $\tilde{\omega}$.

4.2 Exponential Form of the Density Matrix

We now want to calculate correlation functions using the exponential form of the density matrix as in [53]. In [57] the following formula for the thermal average $D_{T,h}^*$ is given

$$D_{T,h}^*(\mathcal{O}) = \dots \frac{1}{2} \text{tr}_1 \frac{1}{2} \text{tr}_2 \frac{1}{2} \text{tr}_3 \dots (e^{\Omega_1 + \Omega_2}(\mathcal{O})) \quad (4.24)$$

where

$$\Omega_1 = \lim_{\alpha \rightarrow 0} \int_{\Gamma} \frac{d\zeta_1^2}{2\pi i \zeta_1^2} \int_{\Gamma} \frac{d\zeta_2^2}{2\pi i \zeta_2^2} \tilde{\omega}(\mu_1, \mu_2; \alpha) \mathbf{b}(\zeta_1, \alpha) \mathbf{c}(\zeta_2, \alpha - 1), \quad (4.25a)$$

$$\Omega_2 = - \lim_{\alpha \rightarrow 0} \int_{\Gamma} \frac{d\zeta_1^2}{2\pi i} \varphi(\mu_1; \alpha) \mathbf{h}(\zeta_1, \alpha). \quad (4.25b)$$

Here Γ is a closed contour around the inhomogeneities ξ_j^2 which excludes all other poles of the integrands and $\mu_j = \ln \zeta_j$. In the homogeneous case Γ encircles only $\zeta^2 = 1$.

Note that there is an error in [53], as the operator Ω_1 should not have the factor -1 occurring there. This is likely a mistake arising from the usage of different conventions. [53] uses the conventions of [50] itself, but builds on [57], which uses the conventions of [49]. During this conversion a factor -1 arises from the product $\mathbf{b}(\zeta, \alpha) \mathbf{c}(\xi, \alpha - 1)$.

The operator $\mathbf{h}(\zeta, \alpha)$ is introduced in [57] in order to accommodate for a magnetic field. More precisely, this operator is needed when calculating the expectation value of an operator uneven under spin reversal in the case of a non-vanishing external field. It is thus clear, that $\mathbf{h}(\zeta, \alpha)$ is needed to define the complete density matrix of the system. We on the other hand restrict ourselves to expectation values of specific operators and can calculate quantities like $\langle \sigma_1^z \sigma_n^z \rangle$ without \mathbf{h} . In the case of uneven operators or operators without a symmetry (like the emptiness formation probability $P(n)$) we only consider the case of a vanishing external field, so we do not need to calculate \mathbf{h} . The reason that \mathbf{h} is not needed in the case of a vanishing field is that the eigenvalue $\Lambda(\zeta, \kappa)$ is even in κ . Then $\varphi(\lambda)$ has to be zero for $\kappa = h = 0$, which means that Ω_2 has to be zero as well. For an operator which is even under spin reversal, i.e. $\mathbb{J}(X) = X$, it follows that $\langle X \rangle_{T,h} = \langle X \rangle_{T,-h}$. Using that ω is an even function in h and φ is an uneven function in h , it follows that any term in $\langle X \rangle_{T,h}$ containing a φ has to vanish. Thus Ω_2 is unneeded in this case as well.

Finally, the reason that the exponential form of the density matrix can be computed efficiently is that the operators Ω_1 and Ω_2 are nilpotent as stated in [53]. We have

$$\Omega_1^{\lfloor n/2 \rfloor + 1} = 0 \quad \text{and} \quad \Omega_2^2 = 0 \quad (4.26)$$

where n is the length of the chain segment. The reason for this is the fermionic nature of the operators $\mathbf{b}(\zeta, \alpha)$ and $\mathbf{c}(\zeta, \alpha)$.

Using the known expansions of the fermionic operators we can express Ω_1 in terms of the modes $\mathbf{b}_i, \mathbf{c}_j$ in the homogeneous case:

$$\Omega_1 = \lim_{\alpha \rightarrow 0} \sum_{i,j=1}^n \frac{\tilde{\omega}^{(i-1,j-1)}(\alpha)}{(i-1)!(j-1)!} \mathbf{b}_i(\alpha) \mathbf{c}_j(\alpha - 1) \quad (4.27)$$

where

$$\tilde{\omega}^{(i,j)}(\alpha) = \partial_{\zeta_1^2}^i \partial_{\zeta_2^2}^j \frac{\tilde{\omega}(\ln \zeta_1, \ln \zeta_2, \alpha)}{\zeta_1^2 \zeta_2^2}. \quad (4.28)$$

To compute the derivatives, we will use (4.23) as before for an easy comparison.
Once Ω_1 is calculated we can compute expectation values using

$$D_{T,h}^*(\mathcal{O}) = \dots \frac{1}{2} \text{tr}_1 \frac{1}{2} \text{tr}_2 \frac{1}{2} \text{tr}_3 \dots \sum_{j=0}^{\lfloor n/2 \rfloor} \frac{\Omega_1^j(\mathcal{O})}{j!} . \quad (4.29)$$

Chapter 5

Construction on the Computer

In this chapter we want to explain how we constructed the fermionic operators on a computer. Once the operators are constructed, we will use them to explicitly compute short-range correlation functions using both techniques discussed in the last chapter.

We will emphasize some problems inherent to the construction and will explain which tests we performed to assure that the results are correct.

5.1 Form

For our computation we used two computer algebra systems, namely Mathematica and Form. We assume that the reader has a basic familiarity with Mathematica. In this section we will briefly introduce Form.

According to their website [59] “FORM is a Symbolic Manipulation System. Its original author is Jos Vermaseren of Nikhef, the Dutch institute for subatomic physics which is part of the Dutch physics granting agency FOM.”

The website contains a documentation and some features are explained in [60].

Compared to Mathematica, FORM is a rather “primitive” language, which will become clear later. This has two advantages for our application. First, FORM is much more efficient than Mathematica when manipulating algebraic expressions like those we will encounter. Efficiency means that it is not only faster but also needs much less memory, which is even more important to us than speed. One of the main reasons for this larger efficiency is that FORM stores expressions serially whereas Mathematica uses more complex trees. This also means that FORM is not able to perform complex manipulations like Mathematica. Secondly, some expressions are actually easier to manipulate in FORM than they are in Mathematica. A good example will be the construction of the operator $\mathbf{k}(\zeta, \alpha)$. To construct this operator explicitly, we will need to handle expressions containing elements of the q -oscillator algebra,

which do not commute. While it is possible to manage non-commuting objects in Mathematica, in FORM such objects are “natural” and thus easier to implement.

In this work we will not go into detail about the language itself. Instead we will provide just a quick and simplified overview of the structure of a typical FORM program. A FORM program consists of a series of modules, which can be viewed as smaller programs which are executed sequentially and share some variables. The basic objects on which a FORM program works are expressions. Each expression is a sum of terms which are stored sequentially in memory. Expressions are defined at the start of a module. After the expressions are defined it is specified how they should be manipulated in the form of executable statements. There are several ways to end a module, but we will restrict ourselves to the “.sort” instruction here. It is the most general end-of-module instruction, telling FORM to execute all expressions and prepare them for the next module. Execution of an expression means that the executable statements of the module are applied to the expression term by term. Since each operation is applied to a single term at a time, it is impossible to do substitutions like $a + b \rightarrow c$ since this would be an operation on two terms. To do this, one would need to use a replacement rule like $a \rightarrow c - b$. After the execution, the resulting terms are brought into a standard form. It is only at this point that trivial simplifications like $a + b - a \rightarrow b$ are done. The reason is simply that for such a simplification it might be necessary to consider more than one term. This makes the placement of end-of-module instructions a delicate matter. Too many .sort instructions will cause a slowdown due to overhead from too much sorting. Not enough .sort instructions will cause terms to be processed which would otherwise cancel out. The proper placement of .sort instructions is often an art by itself. After all expressions are sorted, they are typically inherited by the next module which then continues to process them.

The above can be illustrated by providing a small example for a simple FORM program:

```
1 Symbols a, b, c;
2
3 Local A = (a + b)^3;
4 print;
5 .sort
6
7 id a = c - b;
8 print;
9 .end
```

- Line 1 tells FORM that a , b and c are simple symbols. A symbol is FORMs most basic datatype and generally commutes with everything.

There are other datatypes like “Functions” which do not commute among themselves.

- Line 3 defines a local expression labeled “ A ”. For this example, the distinction between local and global expressions is of no consequence. The expression A will behave as explained above.
- Line 4 lets FORM know that it should print the values of all expressions at the end of the module. The printing generally occurs after sorting the expressions.
- Line 5 marks the end of the current module. Since there was no statement to manipulate A in the module, FORM will just bring A into standard form. This implies working out the brackets.
- Line 7 is an executable statement which does the replacement $a \rightarrow c - b$. It is also the first line of the second module. We do not need to define an expression in this module, since it inherits A from the previous one.
- Line 8 again tells FORM to print out all expressions after sorting.
- Line 9 ends the program. Of course, this ends the current module too, meaning that printing will occur before the program is terminated.

The output of our example program will be

```

Symbols a, b, c;

Local A = (a + b)^3;
print;
.sort

Time =          0.00 sec    Generated terms =          4
          A              Terms in output =          4
                              Bytes used      =          140

A =
  b^3 + 3*a*b^2 + 3*a^2*b + a^3;

id a = c - b;
print;
.end

Time =          0.00 sec    Generated terms =          10
          A              Terms in output =          1

```

Bytes used = 36

```
A =  
  c^3;
```

As one can see, FORM prints out runtime statistics after each module. The expression A is printed after sorting. Internally it is stored as a sequence of 4 terms. The replacement in the second module is then applied to each single term. This causes FORM to generate additional terms which can be seen in the second printout of statistics. During the execution of the replacement the expression A grows to 10 terms which then cancel out during sorting, resulting in a single term in the output.

Before using FORM to construct the fermionic operators it should be noted that FORM can be unstable. Even though FORM is being developed since 1984, it should still be viewed as a work in progress. While using FORM several errors presented themselves in various versions of the program. At the time of this writing (2018/04/05) there are about 60 known errors listed in the official issue tracker at github [61]. At the same time new features are added constantly to the system. Even while using stable releases some errors occurred which could be avoided by using newer commits from github. As a first precaution it seems to be a good strategy to clone the github repository and compile FORM on the machine on which it will be executed. After compilation the automated test suite should be run to test the resulting binaries. Since errors may occur even when using the presented strategy all results should be checked vigorously. Luckily in our case there are plenty of relations which can be tested for every single object constructed. Additionally, the operators build on each other, so testing against known results for correlation functions can be viewed as test for every operator constructed. While working on the construction of the operators another fact presented itself which may boost confidence in our results. Non-trivial relations like reduction and commutativity depend on the correctness of the involved operators in a very sensitive manner. Most of the time even small errors in a program lead to objects which obey none of the checked relations. So, if the operators constructed obey all checked relations they are almost definitely correct.

Lastly, we shall specify the setup that was used for this work. Since FORM relies on many different libraries, it is impractical to document all of them. Instead we will focus on the most important parts. The final version of FORM which was used is compiled from the commit 5721ce5 “[test] Detect another syscall Valgrind error” using gcc 7.3.1. The optional libraries gmp (6.1.2) and zlib (1.2.11) were used.

5.2 Construction of $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$

The operator $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ is the most easy to construct on the computer. This applies to the implementation as well as the required computational work. The program is simply an implementation of formula (2.14).

We will compute the action of $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ on the elements of the canonical basis constructed with the $e_{j\alpha}^\beta$. The program constructs the “innermost” part $q^{\alpha\sigma_a^\pm} X_{[1,n]}$ for each element $X_{[1,n]}$ and then applies the $\mathbb{L}_{a,j}(\zeta)$ one at a time. A sorting occurs after each multiplication. After applying the L matrices, we account for the trace by discarding every term containing a σ_a^+ or σ_a^- .

When $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ is known, the expansion coefficients are obtained by simply calculating

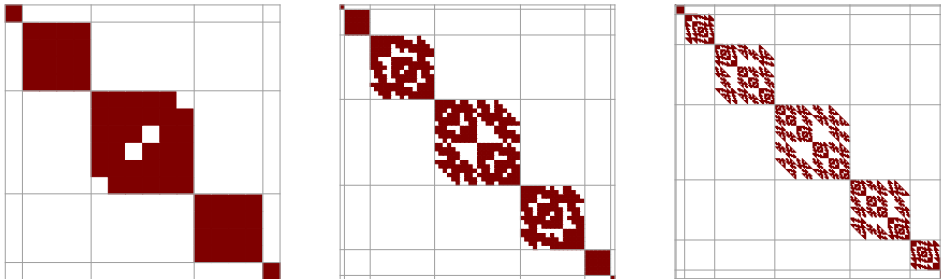
$$\tilde{t}_{j+1}^*(\zeta, \alpha) X_{[1,n]} := \left(\mathbf{t}^*(\zeta, \alpha) - \sum_{p=1}^j t_p^*(\alpha) (\zeta^2 - 1)^{p-1} \right) X_{[1,n]} (\zeta^2 - 1)^{-j} \quad (5.1)$$

and using $t_p^*(\alpha) = \tilde{t}_p^*(1, \alpha)$.

The operator $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ is a good starting point because of its simplicity and the fact that it commutes with virtually every other operator. This provides us with an easy test for the construction of the other operators.

5.2.1 Testing $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$

Before continuing with the other operators, we will test some basic properties of $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ in order to detect possible errors in our program. Since testing does not require much computational work this can be easily done in Mathematica. First, we will plot the operator, colouring every element of the matrix which is not equal to zero. The below example shows $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ for $n = 2, 3, 4$ from left to right. Before plotting, the basis was sorted according to spin. The operators show the expected block structure, since $s(\mathbf{t}_{[1,n]}^*(\zeta, \alpha)) = 0$.



Next, we will test its reduction relations and commutation with itself. We start by testing the left reduction relation. Since \mathbf{t}^* enlarges the support to the right this is very easy to test. An operator $X \in M_{[1,n-1]}$ of length

$\ell(X) = n - 1$ is constructed. On the computer this is represented by a simple list of 4^{n-1} unique symbols. Then

$$\mathbf{t}_{[1,n]}^*(\zeta, \alpha)(q^{\alpha\sigma^z} \otimes X) = q^{\alpha\sigma^z} \otimes \mathbf{t}_{[1,n-1]}^*(\zeta, \alpha)(X) \quad (5.2)$$

is tested. This is repeated for the modes $t_{p,[1,n]}^*(\alpha)$ for $p = 1, \dots, n - 1$.

For the right reduction relation, we will constrict ourselves to the modes $t_{p,[1,n]}^*(\alpha)$. The reason is that the modes are easier to test, because the enlargement of the support is controllable. Additionally, the modes are the objects of interest and not the operator $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ itself. For an operator $X \in M_{[1,n-1]}$ of length $\ell(X) = n - p - 1$ the equation

$$t_{p,[1,n]}^*(\alpha)(X \otimes \text{id}) = t_{p,[1,n-1]}^*(\alpha)(X) \otimes \text{id} \quad (5.3)$$

is tested, where $\text{id} \in M$ is the identity. This is done for $p = 1, \dots, n - 1$.

The last test to check whether $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ and its modes were constructed correctly are the commutation relations. All modes of the transfer matrix should commute with each other. For a given interval length n the commutativity of $t_{p,[1,n]}^*(\alpha)$ and $t_{m,[1,n]}^*(\alpha)$ was tested for all partitions $p + m = n$.

All tests were successful for $n = 2, 3, 4, 5$.

5.3 Construction of $\mathbf{k}_{[1,n]}(\zeta, \alpha)$

The first step in constructing the fermionic operators is the construction of the operator $\mathbf{k}(\zeta, \alpha)$. As discussed before, most of the construction can be done for the case of a finite chain. Since the inductive limit can be done for the annihilation and creation operators, we can treat $\mathbf{k}(\zeta, \alpha)$ on a finite chain. Considering a finite chain of length L , we will construct $\mathbf{k}_{[1,L]}(\zeta, \alpha)$. For our program we changed formula (2.32) in order to express $\mathbf{k}_{\text{skal},[1,L]}$ in terms of the fused L matrices $\mathbb{L}_{\{a,A\},j}$. This can be done since

$$\mathbb{L}_{\{a,A\},j}(X) = F_{a,A}^{-1} \mathbb{L}_{a,j} \mathbb{L}_{A,j}(X) F_{a,A} \quad (5.4)$$

if $[F_{a,A}, X] = 0$ and since $[F_{a,A}, \sigma_a^+] = 0$ and $[F_{a,A}, q^{\alpha(\sigma_a^z + 2D_A)}] = 0$.

Our program uses the formula

$$\begin{aligned} & \mathbf{k}_{\text{skal},[1,L]}(\zeta, \alpha)(X_{[1,L]}) = \\ & \text{tr}_{a,A} \left\{ \sigma_a^+ \mathbb{L}_{\{a,A\},L}(\zeta) \cdots \mathbb{L}_{\{a,A\},1}(\zeta) \left(\zeta^{-2s-1} y^{\sigma_a^z + 2D_A} q^{-2S_{[1,L]}} X_{[1,L]} \right) \right\} \end{aligned} \quad (5.5)$$

where again the operator $X_{[1,L]}$ is of spin s . We will also use $y = q^\alpha$ because it is only a single symbol.

It is then convenient to compute the action of $\mathbf{k}_{\text{skal},[1,L]}(\zeta, \alpha)$ on the canonical basis constructed with the $e_{j\alpha}^\beta$. This will also allow for easy parallelization later.

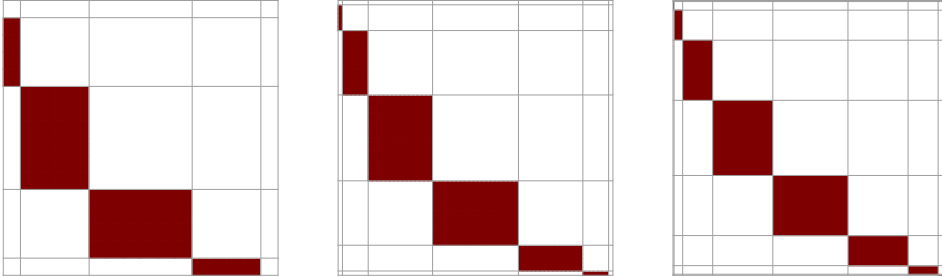
For each element of the basis the “innermost” part

$$\zeta^{-2s-1} q^{\alpha(\sigma_a^z + 2DA)} q^{-2S_{[1,L]}} X_{[1,L]}$$

is constructed first. The spin- $\frac{1}{2}$ auxiliary space is explicitly used, whereas $q^{2\alpha DA}$ is represented by a single non-commuting symbol. Then a single fused L matrix $\mathbb{L}_{\{a,A\},j}(\zeta)$ is applied after which all symbols are commuted and sorted. The bosonic operators are defined in such a way, that they commute with every object but not amongst themselves. In each step a standard ordering of the bosonic operators is enforced. In FORM this is done with statements like `id ad*a = 1 - N^2` or `id N*a = a*N/q`. Following this the sorting process mentioned above occurs, after which the next L matrix is applied. If the loop is finished, the elements e_{a+}^+ , e_{a-}^- and e_{a+}^- can be discarded because of the operator σ_a^+ and the trace tr_a . The remaining trace tr_A can then be taken by discarding all terms which are not “balanced” in \mathbf{a}_A^+ and \mathbf{a}_A and replacing $y^{2DA} q^{mDA} \rightarrow \frac{1}{1-y^2 q^m}$.

5.3.1 Testing $\mathbf{k}_{[1,n]}(\zeta, \alpha)$

As with $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ we will start testing $\mathbf{k}_{[1,n]}(\zeta, \alpha)$ with a matrixplot for $n = 2, 3, 4$.



Since $s(\mathbf{k}_{[1,n]}(\zeta, \alpha)) = 1$ the plots show the expected block structure. The basis is ordered from low to high spin.

Testing the left reduction relation is straight forward. The only difference to $\mathbf{t}_{[1,n]}^*(\zeta, \alpha)$ is that α needs to be shifted since the spin of $\mathbf{k}_{[1,n]}(\zeta, \alpha)$ is not zero. The right reduction relation is more complicated. It is given by lemma 3.4 in [50]:

$$\mathbf{k}_{[k,l]}(\zeta, \alpha)(X_{[k,m]}) = \mathbf{k}(\zeta, \alpha)(X_{[k,m]}) + \Delta_\zeta \mathbf{v}_{[k,l]}(\zeta, \alpha)(X_{[k,m]}) \quad (5.6)$$

where $k \leq m < l$ and $\Delta_\zeta \mathbf{v}_{[k,l]}(\zeta, \alpha)$ is a q -exact operator. We did not undertake the effort to construct $\mathbf{v}_{[k,l]}(\zeta, \alpha)$ on the computer to test this relation in its entirety. Instead, we confirm that the difference $\mathbf{k}_{[k,l]}(\zeta, \alpha)(X_{[k,m]}) - \mathbf{k}(\zeta, \alpha)(X_{[k,m]})$ is q -exact. Since we constructed $\mathbf{k}_{\text{skal},[1,L]}(\zeta, \alpha)$, we expect the difference to be of the form $\zeta^{-\alpha-\mathbb{S}} \Delta_\zeta \zeta^{\alpha+\mathbb{S}} f(\zeta^2)$, i.e. a rational function in ζ^2 with poles in \mathbb{C}^\times only at $\zeta^2 = q^{\pm 2}$.

After testing the reduction relations, we tested the commutation of $\mathbf{k}_{[1,n]}(\zeta, \alpha)$ with the modes $t_{p,[1,n]}^*(\alpha)$. It follows from lemma 4.1 in [50], that

$$\mathbf{k}_{[k,l]}(\xi, \alpha) \mathbf{t}^*(\zeta, \alpha+1)(X_{[k,m]}) \simeq_{\xi} \mathbf{t}_{[k,l]}^*(\zeta, \alpha) \mathbf{k}(\xi, \alpha)(X_{[k,m]}) \pmod{(\zeta^2-1)^{l-m}}. \quad (5.7)$$

Using the mode expansion of $\mathbf{t}^*(\zeta, \alpha)$ we can conclude that

$$\left(\mathbf{k}_{[1,n]}(\zeta, \alpha) t_{p,[1,n]}^*(\alpha+1) - t_{p,[1,n]}^*(\alpha) \mathbf{k}_{[1,n]}(\zeta, \alpha) \right) (X_{[1,n]}) \simeq_{\xi} 0 \quad (5.8)$$

for $p = 1, \dots, n$ where $\ell(X_{[1,n]}) \leq n - p$. Note that the remaining q -exact form may also depend on ζ in this case. It is thus not obvious for which modes of $\mathbf{t}^*(\zeta, \alpha)$ it has to be taken into account. During our tests we made the observation, that the exact form seems to be zero for all $p = 1, \dots, n$. Taking into account the relevant proof of lemma 4.1, we believe that it may be of order $(\zeta^2 - 1)^{l-m}$, or rather $(\zeta^2 - 1)^n$ in our case. This is true for $n = 2, 3, 4$ at least, which was tested explicitly.

All tests mentioned above were successfully conducted for $n = 2, 3, 4$.

5.4 Construction of $\rho_{j,[1,n]}^{(\epsilon)}(\alpha)$ and $\kappa_{j,[1,n]}(\alpha)$

After constructing $\mathbf{k}_{[1,n]}(\zeta, \alpha)$ we will calculate its Laurent coefficients in order to construct the fermionic annihilation operators. To do this $\mathbf{k}_{\text{skal},[1,n]}(\zeta, \alpha)$ is loaded and a loop counts down $j = n, \dots, 1$. For each j we go over $\epsilon = -1, 0, 1$ and set

$$\rho_{j,[1,n]}^{(\epsilon)}(\alpha) = (\zeta^2 - q^{2\epsilon})^j \mathbf{k}_{\text{skal},[1,n]}^{(j,\epsilon)}(\zeta, \alpha) \Big|_{\zeta^2=q^{2\epsilon}} \quad (5.9)$$

$$\kappa_{j,[1,n]}(\alpha) = \zeta^{2j} \mathbf{k}_{\text{skal},[1,n]}^{(j,2)}(\zeta, \alpha) \Big|_{\zeta^2=0} \quad (5.10)$$

where

$$\begin{aligned} \mathbf{k}_{\text{skal},[1,n]}^{(j,\epsilon)}(\zeta, \alpha) &= \mathbf{k}_{\text{skal},[1,n]}(\zeta, \alpha) \\ &- \sum_{k=j+1}^n \sum_{\delta=-1}^{\epsilon-1} \frac{\rho_{k,[1,n]}^{(\delta)}(\alpha)}{(\zeta^2 - q^{2\delta})^k} - \sum_{k=j+1}^n \frac{\kappa_{k,[1,n]}(\alpha)}{\zeta^{2k}}. \end{aligned} \quad (5.11)$$

During traversal of the loop $\kappa_0(\alpha)$ is accumulated which contains all $\rho_j^{(\alpha)}$. Since the $\rho_j^{(0)}$ are only needed for $\kappa_0(\alpha)$ they are discarded as soon as they have entered $\kappa_0(\alpha)$. Each time one of the Laurent coefficients is finished, a sorting is done in order to keep $\mathbf{k}_{\text{skal},[1,n]}^{(j,\epsilon)}(\zeta, \alpha)$ as small as possible.

We do not test the Laurent coefficients directly since they enter the annihilation operators in a simple manner, which are tested thoroughly.

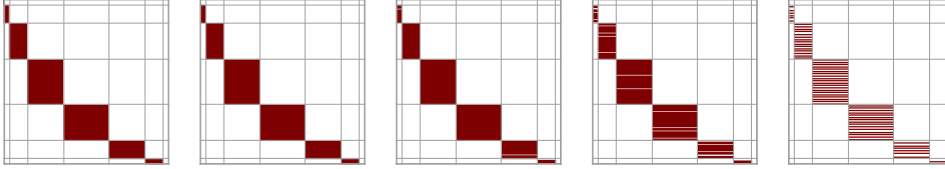
5.5 Construction of the Fermionic Annihilation Operators

Once the Laurent coefficients of $\mathbf{k}_{\text{skal},[1,n]}(\zeta, \alpha)$ are known it is easy to construct the operators $\mathbf{c}_{[1,n]}(\zeta, \alpha)$, $\mathbf{b}_{[1,n]}(\zeta, \alpha)$ and $\mathbf{f}_{[1,n]}(\zeta, \alpha)$. In a loop over $j = 1, \dots, n$ we construct $\mathbf{c}_{j,[1,n]}(\alpha)$ and $\mathbf{f}_{j,[1,n]}(\alpha)$ for every j by combining $\rho_{j,[1,n]}^{(\pm)}$. After they are saved, $\mathbf{f}_{j,[1,n]}(\alpha)$ is discarded to preserve memory and $\mathbf{b}_{j,[1,n]}(\alpha)$ is constructed by applying $\phi(\mathbf{c}_{j,[1,n]}(\alpha))$.

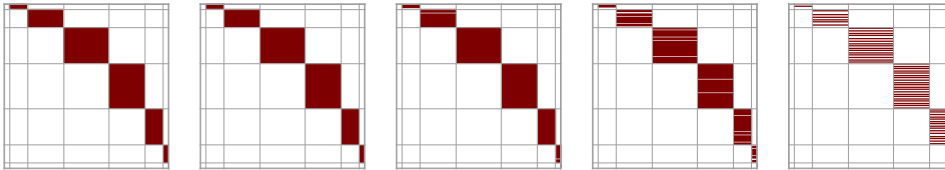
This is done as follows: each term in $\mathbf{c}_{j,[1,n]}(\alpha)$ carries an internal tag to save the according spin which can easily be inverted. The parameter α occurs only indirectly in y . This can be replaced by $y \rightarrow y^{-1}$. The transformation $\mathbb{J}(\cdot)$ can be done easily because of the way we represent matrices. As mentioned before FORM treats every expression as a simple series of terms. In order to represent a matrix, we represent every element as a series of terms which carry tags bra^x and ket^y . The indices x and y are base 4 numbers where we assign 0 to e_+^+ , 1 to e_+^- , 2 to e_-^+ and 3 to e_-^- . The transformation $\mathbb{J}(\cdot)$ can then be achieved simply by replacing $\text{bra}^x \rightarrow \text{bra}^{(4^n - 1 - x)}$ and ket^y accordingly.

5.5.1 Testing the Fermionic Annihilation Operators

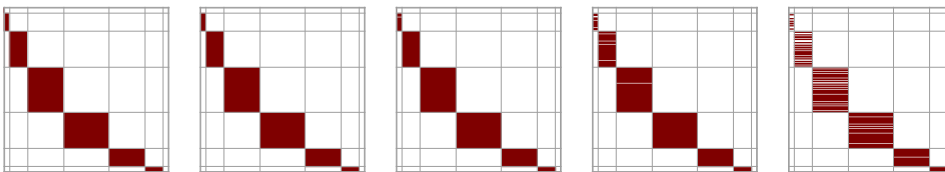
A matrixplot of the operators shows the expected block structure. For the sake of brevity, we only show the plots for $n = 4$. First are the $\mathbf{c}_{j,[1,n]}(\alpha)$, where $j = 0, \dots, 4$ from left to right.



The $\mathbf{b}_{j,[1,n]}(\alpha)$, where $j = 0, \dots, 4$ from left to right:



And the $\mathbf{f}_{j,[1,n]}(\alpha)$, where $j = 0, \dots, 4$ from left to right:



Note that these operators are “thinning out” as j grows. This is intuitively in compliance with the annihilation property.

The left reduction relation given by (2.85) is, of course, the same for all operators, including $\mathbf{f}_{j,[1,n]}(\alpha)$. It is tested for $n = 2, 3, 4$ and $j = 0, \dots, n - 1$ for all three operators.

The right reduction relation is only tested for $\mathbf{c}_{j,[1,n]}(\alpha)$ and $\mathbf{b}_{j,[1,n]}(\alpha)$. This is due to the fact that these two are more important than $\mathbf{f}_{j,[1,n]}(\alpha)$ in the sense that they are used by themselves, whereas $\mathbf{f}_{j,[1,n]}(\alpha)$ only enters in the creation operators which are tested separately. In addition, similar to $\mathbf{k}_{\text{skal},[1,n]}(\zeta, \alpha)$ the right reduction relation for $\mathbf{f}_{j,[1,n]}(\alpha)$ would be more difficult to implement. The reduction for $\mathbf{c}_{j,[1,n]}(\alpha)$ and $\mathbf{b}_{j,[1,n]}(\alpha)$ was given by (2.86).

Next the commutation relations for the annihilation operators are tested. It is tested that all modes of the annihilation operators anticommute with each other (3.23a) and that they commute with the modes of the transfer matrix $t_{p,[1,n]}^*(\alpha)$. Since the annihilation operators preserve the support, we can simply check the anticommutation relations for all combinations of modes. Care has to be taken in the case of the commutation relation with the transfer matrix as explained before.

Another test which can be done for the annihilation operators is to confirm that they obey their name-giving property. For fixed j and $x = c, b$ we confirm that $x_{j,[1,n]}(\alpha)(X_{[1,n]}) = 0$ if $\ell(X_{[1,n]}) < j$.

As before, all tests were conducted for $n = 2, 3, 4$.

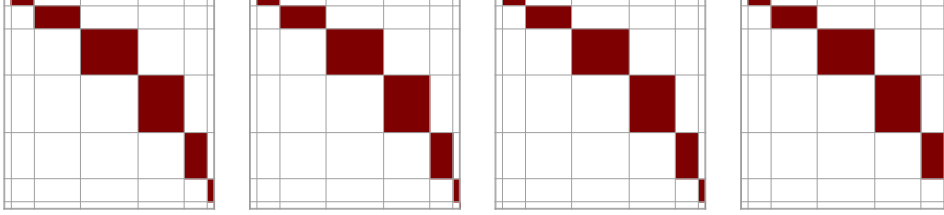
5.6 Construction of the Fermionic Creation Operators

For the creation operators we will construct only the modes $\mathbf{b}_{p,[1,n]}^*(\alpha)$, $\mathbf{c}_{p,[1,n]}^*(\alpha)$ as the generating functions are not needed. First the $\mathbf{b}_{p,[1,n]}^*(\alpha)$ are constructed using (2.81) and then the corresponding modes $\mathbf{c}_{p,[1,n]}^*(\alpha)$ are obtained by applying ϕ (2.22). As before, a loop over all elements of the canonical basis is used which can be executed in parallel. For each element all modes are constructed one at a time. To preserve memory the four sums comprising $\mathbf{b}_{p,[1,n]}^*(\alpha)$ are calculated one after another, loading the needed modes $\mathbf{f}_{j,[1,n]}(\alpha)$ and $\kappa_{j,[1,n]}(\alpha)$ only in a short scope when needed.

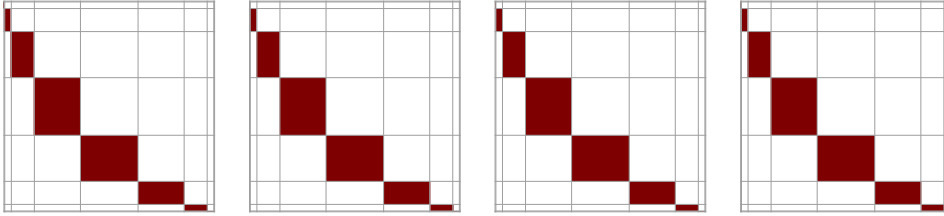
As explained in subsection 3.1.3, there is a subtle difference between operators acting on the finite and infinite chain. This difference becomes important in the case of the creation operators. Up until now it was sufficient to just calculate every operator the way it was explained in chapter 2. In the case of the $\mathbf{b}_{p,[1,n]}^*(\alpha)$ we calculate everything according to chapter 2 as well, but after that compute the alternating sums (3.17) in order to obtain the modes acting on an infinite chain.

5.6.1 Testing the Fermionic Creation Operators

As for the other operators we start with a simple matrixplot for the case $n = 4$. We observe the expected block structure. The following image shows the $\mathbf{c}_{p,[1,n]}^*(\alpha)$, where $p = 1, \dots, 4$ from left to right:



And the next shows the $\mathbf{b}_{p,[1,n]}^*(\alpha)$, where $p = 1, \dots, 4$ from left to right:



In contrast to the annihilation operators we do not observe an increasing number of entries equal to zero with growing p . Again, this is in compliance with our intuition from the support property of the creation operators (2.89).

The modes $\mathbf{b}_{p,[1,n]}^*(\alpha)$, $\mathbf{c}_{p,[1,n]}^*(\alpha)$ have to obey the general left reduction relation (2.85), which is tested for $n = 2, 3, 4$ as for the other operators. The right reduction relation (2.97) is the same as for the modes $t_{p,[1,n]}^*(\alpha)$ and is also tested up to $n = 4$.

For the commutation relations we now can test all remaining relations from (3.23) as well as the commutativity with the modes of the transfer matrix.

5.7 Elements of the Fermionic Basis

In order to use the JMS theorem (4.13) to calculate expectation values, we need to be able to express arbitrary operators $X_{[1,n]} \in M_{[1,n]}$ in terms of the fermionic basis. The first step in achieving this is to construct the elements of the fermionic basis. Following section 3.2 we will first list all the B_J (3.38). This will give us 2^n expressions, which are sums of products of creation operators. At this point the operators are treated as symbols, making the resulting expressions very small. Also the vacuum $q^{2\alpha S(0)}$ is ignored at this point.

The only difficulty in constructing the B_J is the computation of the Littlewood-Richardson coefficients. We developed a small Python script to

construct the B_J where the Littlewood-Richardson coefficients were calculated using a simple backtrack algorithm.

We calculate the coefficients by directly decomposing a product of Schur polynomials: $S_\mu S_\nu = \sum_\lambda c_{\mu,\nu}^\lambda S_\lambda$. Assuming $\mu \supset \nu$ we construct every possible tableau by starting from μ and then filling it one square at a time according to ν . This produces a search tree over all possible ways to write down a diagram of weight ν . Since there is a number of properties that a tableau should obey, we can check every node of the tree for validity, thinning it out considerably. At the lowest level of the tree we can then read out all possible tableaux of shape $\lambda - \mu$ with weight ν such that $w(T)$ is a lattice permutation.

As a simple example we shall compute $B_{\{3,2\}}$ for $n=4$. The sets J, K, I in (3.38) obey $|J| = |K| = |I|$. In our example we have $J = \{3, 2\}$, so $|K| = |I| = 2$. We know that $C_{J,K}^I = c_{\lambda(J),\lambda(K)}^{\lambda(I)}$, where $\lambda(J) = (11)$. The only possible candidates for K are $\{4, 1\}, \{3, 2\}, \{3, 1\}, \{2, 1\}$. This is due to the fact that $\lambda(K)$ is the weight of all tableaux and thus $|\lambda(K)|$ has to be the number of squares of each tableau. Additionally, we know that $\lambda(I) - \lambda(J)$ has to be the shape of each tableau and therefore $|\lambda(I) - \lambda(J)|$ also has to be equal to the number of squares. Since J is known, we can conclude that $|\lambda(I) - \lambda(J)| \leq 2$ and therefore $|\lambda(K)| \leq 2$.

We will now construct every possible tableau for each candidate for K . Choose $K = \{4, 1\}$, i.e $\lambda(K) = (2)$. We have to append two squares with number 1 to the basic diagram

$$\begin{array}{|c|} \hline 0 \\ \hline 0 \\ \hline \end{array} .$$

Obviously, the squares with number 0 will be ignored when considering the shape of the tableau. The number of possible choices for ‘‘filling’’ this diagram can be reduced by constricting the diagram to have a maximum of two rows and two columns. More than two rows would require $|I| > 2$ and more than two columns would correspond to indices greater than 4. The only possible diagram remaining is

$$\begin{array}{|c|c|} \hline 0 & 1 \\ \hline 0 & 1 \\ \hline \end{array}$$

which is not a tableau since the numbers other than 0 are not increasing strictly down each column. This means there is no $C_{J,K}^I \neq 0$ for $K = \{4, 1\}$. The choices $K = \{3, 2\}, \{3, 1\}$ lead to one possible diagram each:

$$\begin{array}{|c|c|} \hline 0 & 2 \\ \hline 0 & 1 \\ \hline \end{array} \quad \begin{array}{|c|c|} \hline 0 & 1 \\ \hline 0 & \\ \hline \end{array} .$$

Both of these are valid tableaux and therefore $C_{\{3,2\},K}^I = 1$ for $I = \{4, 3\}, \{4, 2\}$ respectively. This leads to the combinations $\mathbf{c}_3^* \mathbf{c}_2^* \mathbf{b}_2^* \mathbf{b}_1^*$ and $\mathbf{c}_3^* \mathbf{b}_3^* \mathbf{c}_1^* \mathbf{b}_1^*$.

Only the choice $K = \{2, 1\}$ remains. But since $\lambda(K) = \emptyset$ and $c_{\mu, \emptyset}^\lambda = \delta_{\mu}^\lambda$ we already know that the only contribution in this case is for $I = J = \{3, 2\}$, i.e. $\mathbf{b}_4^* \mathbf{c}_2^* \mathbf{c}_1^* \mathbf{b}_1^*$ with a coefficient of one.

It follows that

$$B_{\{3,2\}} = \mathbf{c}_3^* \mathbf{c}_2^* \mathbf{b}_2^* \mathbf{b}_1^* + \mathbf{c}_3^* \mathbf{b}_3^* \mathbf{c}_1^* \mathbf{b}_1^* + \mathbf{b}_4^* \mathbf{c}_2^* \mathbf{c}_1^* \mathbf{b}_1^* . \quad (5.12)$$

Once we have calculated all B_J it is simple to obtain all basis elements using (3.48). The same script that generates the B_J also prepends all possible $\bar{\mathbf{b}}_M$ and \mathbf{c}_N . We then import these combinations into a small FORM program to apply the commutation relations, obtaining all elements of the fermionic basis.

All calculations described in this section can be done very quickly on a normal laptop and thus do not require much optimization. Even for $n = 5$ the calculations take only about one second. Obtaining the basis elements as explicit operators, i.e. inserting the explicit forms of the creation operators, on the other hand takes considerably longer. The obvious way to achieve this is to go through each basis element term by term. For each term we apply the creation operators to the vacuum one after another from right to left, reducing intermediate results to simple operators in $M_{[1,n]}$ instead of End $M_{[1,n]}$.

5.8 Change of Basis

After calculating the basis elements explicitly we now can express arbitrary operators $X_{[1,n]} \in M_{[1,n]}$ in terms of the fermionic basis. As mentioned, this is used to obtain expectation values of such operators using the JMS theorem.

Since the change of basis requires only the solution of a linear system of equations, we will not explain the calculation here. It should suffice to mention that the solution was implemented in FORM in order to save memory.

5.9 Expectation Values of Basis Elements

We will now compute expectation values of the elements of the fermionic basis, which is also done in Form. First the elements of the fermionic basis are imported. Here we do not use the explicit form which is only needed to perform the change of basis, but rather treat the creation operators as symbols. Since we are interested in the spin zero sector, we only consider elements of the basis which have equally many \mathbf{b}_p^* and \mathbf{c}_p^* .

The modes \mathbf{t}_p^* of the transfer matrix can be treated easily by replacing them according to (4.22) and (4.23):

$$\mathbf{t}_p^* \rightarrow \frac{2}{(p-1)!} \sum_{k=0}^{n-1} B_0(n-1, k) \rho^{(k)} \quad (5.13)$$

where $\rho^{(k)} = \partial_\lambda \rho(\lambda)|_{\lambda=0}$. We then expand ρ in α , meaning we replace

$$\rho^{(k)} \rightarrow \delta_{k,0} + \alpha \eta \varphi^{(k)} . \quad (5.14)$$

The determinant is then constructed using simple symbols \mathfrak{D}_{ij} , identifying

$$\mathbf{b}_{r_1}^* \cdots \mathbf{b}_{r_l}^* \mathbf{c}_{s_1}^* \cdots \mathbf{c}_{s_l}^* \hat{=} \det(\mathfrak{D}_{r_i, s_j})_{i,j=1, \dots, N} \quad (5.15)$$

which keeps all expressions very small in terms of memory consumption.

Since FORM is a primitive language, it can not be used to compute such a determinant with a predefined statement. Therefore we will use a simple substitution scheme to compute the determinant according to Leibniz's rule $\det A = \epsilon_{i_1, \dots, i_n} a_{1, i_1} \cdots a_{n, i_n}$.

We will first substitute

$$\mathbf{b}_{r_1}^* \cdots \mathbf{b}_{r_l}^* \mathbf{c}_{s_1}^* \cdots \mathbf{c}_{s_l}^* \rightarrow (\mathbf{b}_{r_1}^* \mathbf{c}_{s_1}^* \cdots \mathbf{c}_{s_l}^*) (\mathbf{b}_{r_2}^* \mathbf{c}_{s_1}^* \cdots \mathbf{c}_{s_l}^*) \cdots (\mathbf{b}_{r_l}^* \mathbf{c}_{s_1}^* \cdots \mathbf{c}_{s_l}^*) . \quad (5.16)$$

After that we will apply the rule

$$\mathbf{b}_r^* \mathbf{c}_{s_1}^* \cdots \mathbf{c}_{s_l}^* \rightarrow e(s_1) \mathfrak{D}_{r, s_1} \cdots e(s_l) \mathfrak{D}_{r, s_l} . \quad (5.17)$$

Note that the functions e , like the fermionic operators, are chosen to be non-commuting, so that their order will be preserved. At this point it only remains to replace the functions e with the Levi-Civita symbol

$$e(s_1) \cdots e(s_l) \rightarrow \epsilon_{s_1, \dots, s_l} , \quad (5.18)$$

thus obtaining the Leibniz formula.

At last we will replace the symbols \mathfrak{D} according to (4.22):

$$\mathfrak{D}_{r_i, s_j} \rightarrow \frac{\partial^{r_i-1}}{(\zeta_i^+)^2} \frac{\partial^{s_j-1}}{(\zeta_j^-)^2} \tilde{\omega}(\ln \zeta_i^+, \ln \zeta_j^-) \Bigg|_{(\zeta_i^+)^2 = (\zeta_i^-)^2 = 1} \quad (5.19)$$

and expand ω in α :

$$\tilde{\omega} \rightarrow \tilde{\omega} + \alpha \tilde{\omega}' . \quad (5.20)$$

5.10 Construction of Ω_1

As presented before, when using the exponential form of the density matrix we will confine ourselves to the case of operators which are even under spin reversal or to a vanishing external field. In this case we will only need Ω_1 to calculate the action of the density matrix. Expectation values are then obtained by

$$\langle \mathcal{O} \rangle_{T,h} = \frac{1}{2^n} \text{tr}_{[1,\dots,n]} \left(\sum_{j=0}^{\lceil n/2 \rceil} \frac{\Omega_1^j}{j!} \mathcal{O} \right). \quad (5.21)$$

In order to save memory, we will not compute the Ω_1^j explicitly. Instead we will only compute the action of these operators on \mathcal{O} .

Our program performs a loop over the powers of Ω_1 . During the first run we calculate $\Omega_1 \mathcal{O}$ and save this vector as \mathcal{O}_1 . Subsequent runs then obtain $\Omega_1 \mathcal{O}_j$. Considering (4.27) it is clear that the factor $\tilde{\omega}^{(ij)}$ contains the information which of the annihilation operators were applied to each term. In other words: given a vector \mathcal{O}_j , the symbols $\tilde{\omega}^{(ij)}$ tell us which combinations of annihilation operators generated a given term in this vector. Because of this we can filter out irrelevant terms in each subsequent run by observing the prefactors. By irrelevant we mean terms which contain a specific annihilation operator at least twice. These will of course drop out since the annihilators are fermionic. Namely, when executing the double sum in (4.27) for a step $\Omega_1 \mathcal{O}_j$ we can, for every (i, j) , discard terms that already contain $\tilde{\omega}^{(i-1,*)}$ or $\tilde{\omega}^{(*,j-1)}$.

After computing every term of the sum in (5.21) we take the trace, which requires a bit of housekeeping in Form. The reason is that \mathcal{O}_j are interpreted as vectors and are internally stored as sequences of terms. Each term carries a tag, specifying to which element of the vector that term belongs. However, it can easily be derived which elements of the vector need to be discarded. Taking the trace is then done by filtering all terms for their appropriate tags.

The expansion of the $\tilde{\omega}^{(ij)}$ according to (4.23) is done at the very last step of the FORM program. Taking the limit $\alpha \rightarrow 0$ is then done in Mathematica, since it proves difficult to handle in Form. At this point the use of Mathematica no longer poses a problem, since the expressions are small enough to be handled by it.

5.11 Parallelization

As mentioned before, the construction of the fermionic operators as well as further calculations using these operators require much computational effort. This becomes obvious if one considers that each operator consists of 16^n elements, each of which is a rational function in q and y . Of course, these rational functions themselves grow with increasing n . As an example consider

the operator \mathbf{b}^* . We measure the required disc space for all modes of the operator depending on n :

n	Size of Files
1	187 B
2	15 KiB
3	764 KiB
4	29 MiB
5	937 MiB

If we want to calculate expectation values for “big” systems, in our case meaning interval lengths > 4 , the question of parallelization naturally arises.

The action of all of the above operators on each element of the canonical basis $e_{j\alpha}^\beta$ is calculated separately which is the natural strategy for linear maps. This approach already allows us a massive parallelization of our computational work. Most calculations can be split into 4^n parts, which is sufficient for our purposes. However, if we want to distribute computations among several computers, some kind of load balancing is needed, since the required work can differ greatly depending on the chosen basis element. In our test we observed that without active load balancing choosing a power of 2 for the number of jobs results in an extremely unbalanced load distribution. The reason is most likely the block structure of the fermionic operators with regard to spin. This results in jobs, which require very different amounts of computation time. Choosing a prime number will yield much better results.

Later we chose to additionally use an existing system for active load balancing, namely GNU Parallel [62]. Parallel is a tool that can distribute jobs to several machines on demand and thus ensure that all machines are fully used at all times. Another advantage of using this system is that issuing jobs to multiple machines becomes much easier since less manual intervention is needed. Of course, even with an active load balancing it is still beneficial to choose a prime number of jobs.

5.12 Prospects for the Case $n = 6$

In the context of this work all fermionic operators were constructed for lengths up to $n = 5$. Also, the algebraic parts of the correlation functions $\langle \sigma_1^x \sigma_n^x \rangle$ and $\langle \sigma_1^z \sigma_n^z \rangle$ have been computed up to the same length. We believe that in principle it would be possible to calculate these objects for length $n = 6$ in several weeks using our programs on moderate hardware, meaning ~ 10 consumer grade PCs. The difficulty that prevented this calculation in the context of this work was that FORM uses a complicated setup of various buffers and scratch files. The size of these needs to be set before a program is run. However, if these setup parameters are chosen insufficiently the program will at some point terminate unsuccessfully. Since the memory usage of the

programs depends on the setup of buffer sizes, it is not practical to just choose very large buffers. To construct the case $n = 6$ one would need to spend some additional time to find sufficient settings or a machine with a large amount of memory. Sadly, we did not have access to such a machine for interactive testing.

5.13 The Function ω

In order to obtain numerical values for the functions ω and ω' we use a program that was developed by Michael Brockmann and Jens Damerau in C. Later it received an update by Alexander Weiße which made sure that it no longer depended on old and proprietary libraries. This is also the program which was used in [53].

The program in question has a long and convoluted development history and was used to compute numerous different quantities. For our purposes it was therefore necessary to review parts of the code and to make some small changes. With these changes the program now prints out a table which contains the two functions ω and ω' as well as their derivatives using a simple CSV format that can be read by other programs like Mathematica.

The integrations performed by the program depend on two parameters passed to it on execution: the number of points to use and the integration interval, i.e. the cut-off to use. It should be noted that these two parameters are not completely independent. Enlarging the interval while using the same number of points reduces the “effective resolution” used for the integration. Thus, the precision can decline when choosing a bigger interval. Since the program provides no error control it is important to find some measure of the numerical quality of the results. This importance is easily emphasized when naively trying some integration parameters, since this quickly leads to obviously wrong correlation functions like the example shown in figure 5.1. These plots are shown in anticipation of the next chapter. Our goal here is simply to illustrate how the numerical errors in $\omega^{(l)}$ and their derivatives enter into the final results. The two conventions used in the figure refer to the derivatives of the functions ω and ω' . The x -convention always uses derivatives $\omega_{ij}^{(l)}$ where $i \geq j$ and the y -convention uses $i \leq j$. In other words one can obtain the y -graphs by taking the x -graphs and then substituting $\omega_{ij} \rightarrow \omega_{ji}$ and $\omega'_{ij} \rightarrow -\omega'_{ji}$. It is therefore clear that both conventions are equivalent and all differences have to be caused by numerical errors.

Our first strategy for the choice of both parameters was the following: We considered the non-linear integral equations (NLIEs) solved within the program in order to obtain the auxiliary functions \mathfrak{b} and $\bar{\mathfrak{b}}$ which are given in equations (52), (53) of [53]. We shall write down these NLIEs for convenience:

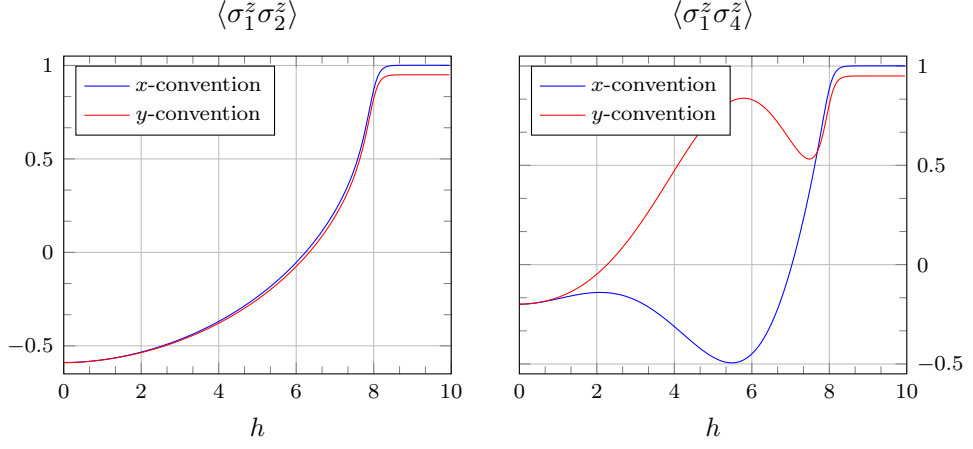


Figure 5.1: Correlation functions for $n = 2$ and $n = 4$ using two equivalent conventions for ω with $\Delta = 0.995$ and $T/J = 0.1$. Integration parameters are 2^{14} points and cut-off $C = 20$.

$$\begin{aligned} \ln \mathfrak{b}(x) = & -\frac{\pi h}{2(\pi - \gamma)T} - \frac{2\pi J \sin(\gamma)}{T\gamma \operatorname{ch}(\pi x/\gamma)} + \int_{-\infty}^{\infty} \frac{dy}{2\pi} F(x-y) \ln(1 + \mathfrak{b}(y)) \\ & - \int_{-\infty}^{\infty} \frac{dy}{2\pi} F(x-y + \eta^-) \ln(1 + \bar{\mathfrak{b}}(y)) \end{aligned} \quad (5.22a)$$

$$\begin{aligned} \ln \bar{\mathfrak{b}}(x) = & \frac{\pi h}{2(\pi - \gamma)T} - \frac{2\pi J \sin(\gamma)}{T\gamma \operatorname{ch}(\pi x/\gamma)} + \int_{-\infty}^{\infty} \frac{dy}{2\pi} F(x-y) \ln(1 + \bar{\mathfrak{b}}(y)) \\ & - \int_{-\infty}^{\infty} \frac{dy}{2\pi} F(x-y - \eta^-) \ln(1 + \mathfrak{b}(y)) \end{aligned} \quad (5.22b)$$

where $\gamma = -i\eta \in \mathbb{R}$, $\eta^- = \eta - i\epsilon$ and

$$F(x) = \int_{-\infty}^{\infty} dk \frac{\operatorname{sh}((\pi - 2\gamma)k/2) e^{ikx}}{2\operatorname{sh}((\pi - \gamma)k/2) \operatorname{ch}(\gamma k/2)}. \quad (5.23)$$

We choose to consider these equations because it seems plausible that they would be the most difficult to solve. All other integral equations solved within the program are linear and therefore should be less difficult to solve. The asymptotic behaviour of the auxiliary functions is known to be $\mathfrak{b} \sim e^{-h/T}$ and $\bar{\mathfrak{b}} \sim e^{h/T}$ for $|x| \gg 1$ (see chap. 13 in [3]). As we will see later there are considerable numerical difficulties for certain sets of parameters, e.g. $\Delta = 0.995$, $h = 5$ and $T/J = 0.1$. For this choice of Δ the asymptotic behaviour of $F(x)$ can easily be determined to be

$$F(x) \sim \frac{2\pi}{\pi - \gamma} \tan\left(\frac{\gamma\pi}{\pi - \gamma}\right) e^{-\frac{2\pi}{\pi - \gamma}|x|}.$$

For a sufficiently large cut-off C we can therefore estimate the error of a single integration to be

$$\epsilon(C) = 2 \ln \left(1 + e^{h/T} \right) \int_C^\infty \frac{dy}{2\pi} F(y) = \frac{\ln \left(1 + e^{h/T} \right)}{\pi} \tan \left(\frac{\gamma\pi}{\pi - \gamma} \right) e^{-\frac{2\pi}{\pi - \gamma} C} .$$

Even with the parameters presented above, the error of an integration becomes as small as the machine precision ($\sim 10^{-16}$) when choosing a relatively small cut-off $C \geq 18$. Considering figure 5.1 however it is clear that this cut-off is insufficient for the procedure as a whole. It should be noted that increasing the number of discretization points leaves the figure completely unchanged. Also, considering the order of magnitude of the errors, a proliferation during the iterative solution is likely not the dominant error source, since the observed errors still depend on the chosen cut-off.

After these considerations we assume that the dominant numeric errors arise in the “higher order” integral equations (54)–(63) presented in [53]. Since the analysis of these would be much more involved, we moved to a more direct and pragmatic measure of numerical quality. Due to the symmetry of ω and ω' we know that the following functions have to be zero:

$$\omega'_{ii} = 0, \quad \Delta\omega_{ij} = \omega_{ij} - \omega_{ji} = 0, \quad \Delta\omega'_{ij} = \omega'_{ij} + \omega'_{ji} = 0 .$$

Thus, any non-zero value of these functions indicates numerical errors. In figure 5.2, such errors are shown for three different derivatives of ω' . It immediately seems plausible that such errors would lead to the behaviour shown in figure 5.1. Like above, increasing the number of discretization points does not change any of the graphs in figure 5.2. The same type of error does not appear in the function ω . Figure 5.3 shows one derivative of ω as an example. The graphs shows that the relative errors are of the order of magnitude of the machine precision. This explains why there are clearly discretization steps in the error graph. We shall call the errors shown in figure 5.2 errors of type one. These errors only appear in derivatives of ω' and do not depend on the number of discretization points. We verified this for all functions $\omega_{ij}^{(l)}$ where $i, j \leq 4$. Instead, errors of type one only depend on the chosen cut-off C . Here the error is inversely proportional to C , i.e. doubling C halves the error.

Up until now we used an abundant number of integration points for all graphs. Meaning that the effective resolution, i.e. the number of points divided by the interval length was high enough so that only errors of type one would emerge. We shall now show what happens if we increase C further while using the same number of discretization points. It is to be expected that at some point numerical errors emerge because the effective resolution will decrease. Figure 5.4 shows how plateaus emerge in the function ω if the resolution becomes too low. These plateaus also emerge in ω' and all derivatives. Such plateaus will also appear in the correlation functions but

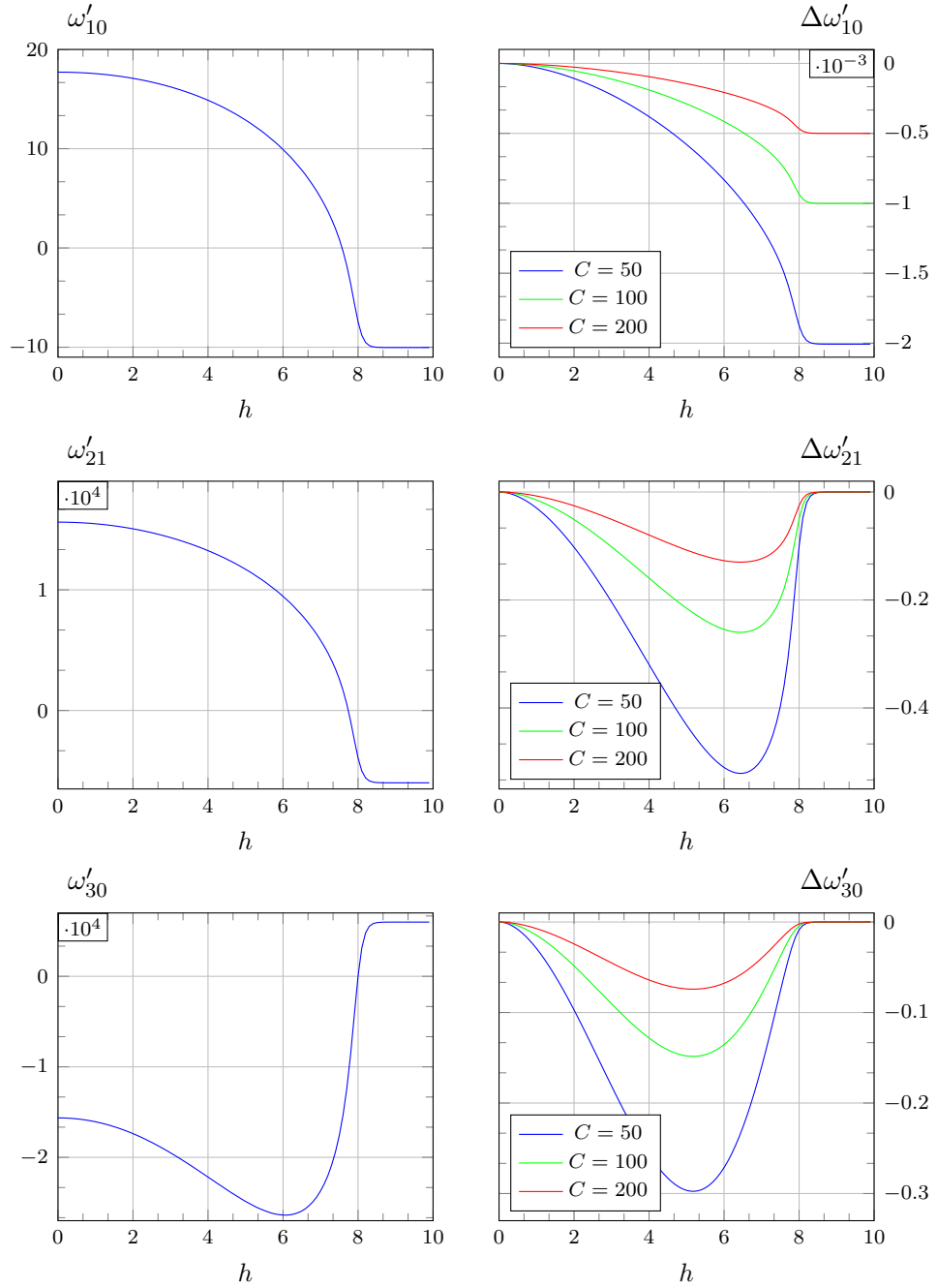


Figure 5.2: Some derivatives of ω' as well as their errors for different cut-offs using $\Delta = 0.995$, $T/J = 0.1$ and 2^{17} discretization points. In the left column the graphs for all three choices of C coincide.

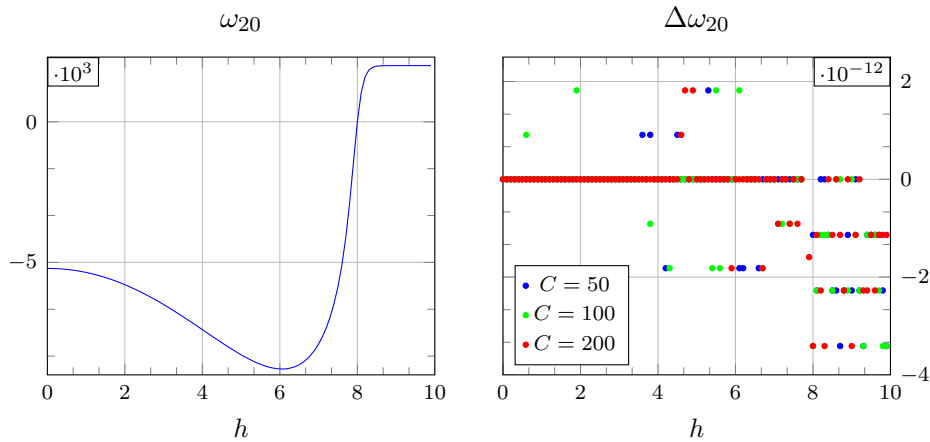


Figure 5.3: The function ω_{20} as well as its numerical errors for different cut-offs using $\Delta = 0.995$, $T/J = 0.1$ and 2^{17} discretization points. Like before, in the left picture the graphs for different cut-offs coincide.

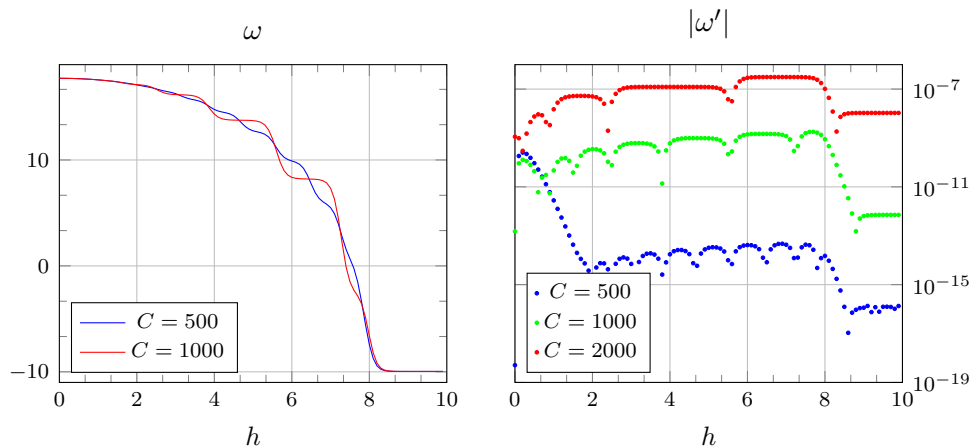


Figure 5.4: The functions ω and ω' at insufficient resolutions. $\Delta = 0.995$, $T/J = 0.1$ and 2^{17} points.

may be more subtle there and are best observed by considering $\omega^{(l)}$ and its derivatives directly. The function ω' should be equal to zero. Here we can observe the expected behaviour: increasing C means reducing the effective resolution and thus increasing the error. We shall call these errors of type two.

Figure 5.5 finally shows some examples of functions for different numbers of discretization points. The function ω'_{11} shows the expected behaviour. ω_{10} seems to be equal to zero as its modulus decreases with an increasing resolution. There are various derivatives of ω showing this behaviour. The figure confirms that errors of type one do not depend on the resolution. One

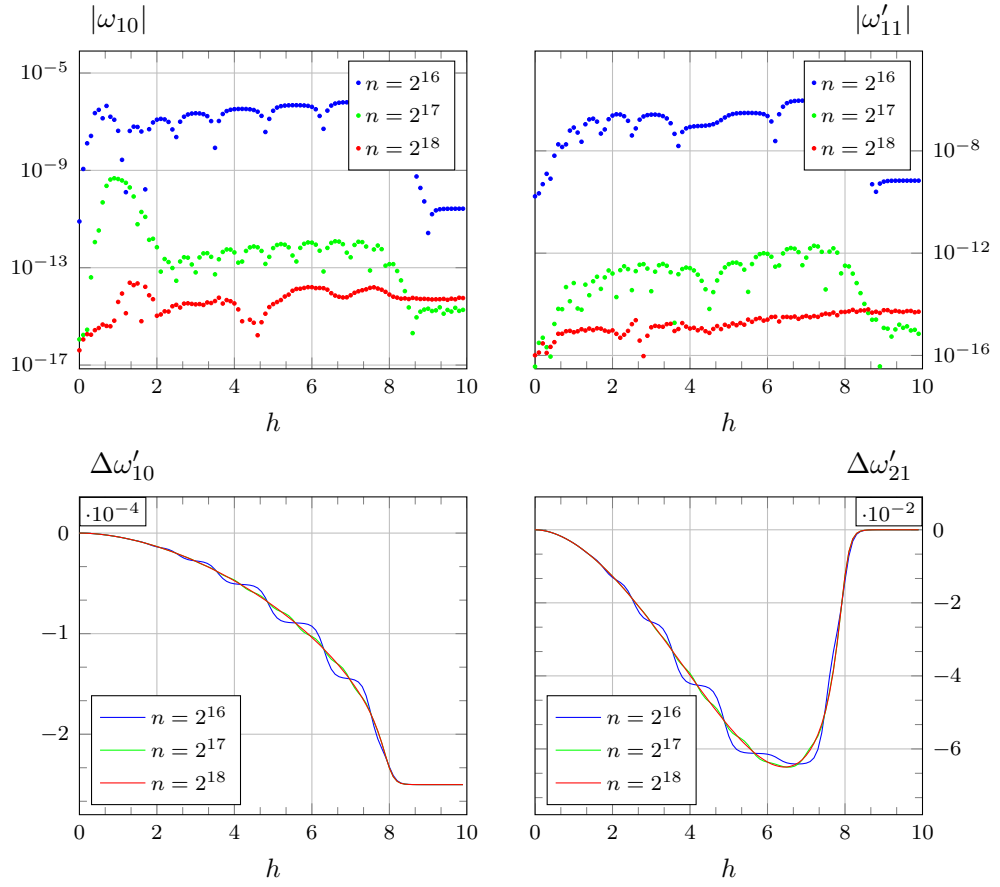


Figure 5.5: Errors of derivatives of ω and ω' for different numbers of discretization points (n), $C = 400$, $T/J = 0.1$, $\Delta = 0.995$.

can clearly see that plateaus emerge in the differences $\Delta\omega'_{10}$ and $\Delta\omega'_{21}$ but their order of magnitude does not change with the resolution.

As we will see in the next chapter, in order to obtain the desired correlation functions we need to insert ω and its derivatives into complicated rational expressions. This is best demonstrated by the correlation functions for $n = 5$ shown in appendix B. Therefore, the question remains how the errors of ω and its derivatives enter into the final results. This will be discussed in section 6.3 along with the results.

Chapter 6

Results of the Computation

Here we will present the results of our calculations on the computer. After addressing both methods of obtaining correlation functions, we will show the functions themselves and compare our results with other works.

6.1 JMS Theorem

In this section we shall show the results of the computation using the JMS theorem. First, we will show the obtained elements for the fermionic basis for several interval lengths. After that we will solve the linear system of equations needed to express a given operator in terms of the fermionic basis. Lastly, we shall show some correlation functions and other expectation values obtained through the JMS theorem. In this section we will only compare our results with [53]. Comparisons with other works are done in the next two sections.

6.1.1 Elements of the Fermionic Basis

As explained above, the elements of the fermionic basis are calculated using a Python script and a small FORM program. Here we will show the results of these computations. For brevity we shall omit writing $q^{2\alpha S(0)}$ in this section. Every element shown is to be applied to this operator. For $n = 1$ there are just four simple elements:

$$\mathbf{b}_1^*, \quad \mathbf{t}_1^*, \quad \mathbf{c}_1^*, \quad 1 .$$

The case $n = 2$ can be compared to [51]. Note that there is an error in an early version of this paper which was later corrected. There are 16 elements

$$\begin{aligned} & \mathbf{b}_2^* \mathbf{b}_1^*, \quad \mathbf{b}_1^* \mathbf{t}_2^* - \mathbf{b}_2^* \mathbf{t}_1^*, \quad \mathbf{b}_1^* \mathbf{t}_1^*, \quad (\mathbf{t}_1^*)^2, \quad \mathbf{c}_2^* \mathbf{b}_1^* + \mathbf{b}_2^* \mathbf{c}_1^*, \quad \mathbf{b}_2^*, \\ & \mathbf{c}_1^* \mathbf{t}_2^* - \mathbf{c}_2^* \mathbf{t}_1^*, \quad \mathbf{t}_2^*, \quad \mathbf{c}_1^* \mathbf{b}_1^*, \quad \mathbf{b}_1^*, \quad \mathbf{c}_1^* \mathbf{t}_1^*, \quad \mathbf{t}_1^*, \quad \mathbf{c}_2^* \mathbf{c}_1^*, \\ & \mathbf{c}_2^*, \quad \mathbf{c}_1^*, \quad 1 . \end{aligned}$$

The case $n = 3$ is already much more complicated, as expected. The 64 elements are

$$\begin{aligned}
& \mathbf{b}_3^* \mathbf{b}_2^* \mathbf{b}_1^*, \quad \mathbf{b}_2^* \mathbf{b}_1^* \mathbf{t}_3^* - \mathbf{b}_3^* \mathbf{b}_1^* \mathbf{t}_2^* + \mathbf{b}_3^* \mathbf{b}_2^* \mathbf{t}_1^*, \quad \mathbf{b}_2^* \mathbf{b}_1^* \mathbf{t}_2^* - \mathbf{b}_3^* \mathbf{b}_1^* \mathbf{t}_1^*, \quad \mathbf{b}_2^* \mathbf{b}_1^* \mathbf{t}_1^*, \\
& \mathbf{b}_1^* \mathbf{t}_1^* \mathbf{t}_3^* - \mathbf{b}_1^* (\mathbf{t}_2^*)^2 + \mathbf{b}_2^* \mathbf{t}_1^* \mathbf{t}_2^* - \mathbf{b}_3^* (\mathbf{t}_1^*)^2, \quad \mathbf{b}_1^* \mathbf{t}_1^* \mathbf{t}_2^* - \mathbf{b}_2^* (\mathbf{t}_1^*)^2, \\
& \mathbf{b}_1^* (\mathbf{t}_1^*)^2, \quad (\mathbf{t}_1^*)^3, \quad \mathbf{c}_3^* \mathbf{b}_2^* \mathbf{b}_1^* + \mathbf{b}_3^* \mathbf{c}_2^* \mathbf{b}_1^* + \mathbf{b}_3^* \mathbf{b}_2^* \mathbf{c}_1^*, \quad \mathbf{b}_3^* \mathbf{b}_2^*, \\
& \mathbf{c}_2^* \mathbf{b}_1^* \mathbf{t}_3^* - \mathbf{c}_3^* \mathbf{b}_1^* \mathbf{t}_2^* + \mathbf{c}_3^* \mathbf{b}_2^* \mathbf{t}_1^* + \mathbf{b}_2^* \mathbf{c}_1^* \mathbf{t}_3^* - \mathbf{b}_3^* \mathbf{c}_1^* \mathbf{t}_2^* + \mathbf{b}_3^* \mathbf{c}_2^* \mathbf{t}_1^*, \\
& \mathbf{b}_2^* \mathbf{t}_3^* - \mathbf{b}_3^* \mathbf{t}_2^*, \quad \mathbf{c}_2^* \mathbf{b}_1^* \mathbf{t}_2^* - \mathbf{c}_3^* \mathbf{b}_1^* \mathbf{t}_1^* + \mathbf{b}_2^* \mathbf{c}_1^* \mathbf{t}_2^* - \mathbf{b}_3^* \mathbf{c}_1^* \mathbf{t}_1^*, \\
& \mathbf{b}_2^* \mathbf{t}_2^* - \mathbf{b}_3^* \mathbf{t}_1^*, \quad \mathbf{c}_1^* \mathbf{t}_1^* \mathbf{t}_3^* - \mathbf{c}_1^* (\mathbf{t}_2^*)^2 + \mathbf{c}_2^* \mathbf{t}_1^* \mathbf{t}_2^* - \mathbf{c}_3^* (\mathbf{t}_1^*)^2, \\
& \mathbf{t}_1^* \mathbf{t}_3^* - (\mathbf{t}_2^*)^2, \quad \mathbf{c}_2^* \mathbf{b}_2^* \mathbf{b}_1^* + \mathbf{b}_3^* \mathbf{c}_1^* \mathbf{b}_1^*, \quad \mathbf{b}_3^* \mathbf{b}_1^*, \\
& \mathbf{c}_1^* \mathbf{b}_1^* \mathbf{t}_3^* - \mathbf{c}_2^* \mathbf{b}_1^* \mathbf{t}_2^* + \mathbf{c}_2^* \mathbf{b}_2^* \mathbf{t}_1^* + \mathbf{b}_3^* \mathbf{c}_1^* \mathbf{t}_1^*, \quad \mathbf{b}_1^* \mathbf{t}_3^* - \mathbf{b}_3^* \mathbf{t}_1^*, \\
& \mathbf{c}_1^* \mathbf{b}_1^* \mathbf{t}_2^* - \mathbf{c}_2^* \mathbf{b}_1^* \mathbf{t}_1^*, \quad \mathbf{b}_1^* \mathbf{t}_2^*, \quad \mathbf{c}_1^* \mathbf{t}_1^* \mathbf{t}_2^* - \mathbf{c}_2^* (\mathbf{t}_1^*)^2, \quad \mathbf{t}_1^* \mathbf{t}_2^*, \\
& \mathbf{c}_1^* \mathbf{b}_2^* \mathbf{b}_1^*, \quad \mathbf{b}_2^* \mathbf{b}_1^*, \quad \mathbf{c}_1^* \mathbf{b}_1^* \mathbf{t}_2^* - \mathbf{c}_1^* \mathbf{b}_2^* \mathbf{t}_1^*, \quad \mathbf{b}_1^* \mathbf{t}_2^* - \mathbf{b}_2^* \mathbf{t}_1^*, \\
& \mathbf{c}_1^* \mathbf{b}_1^* \mathbf{t}_1^*, \quad \mathbf{b}_1^* \mathbf{t}_1^*, \quad \mathbf{c}_1^* (\mathbf{t}_1^*)^2, \quad (\mathbf{t}_1^*)^2, \quad \mathbf{c}_3^* \mathbf{c}_2^* \mathbf{b}_1^* + \mathbf{c}_3^* \mathbf{b}_2^* \mathbf{c}_1^* + \mathbf{b}_3^* \mathbf{c}_2^* \mathbf{c}_1^*, \\
& \mathbf{c}_3^* \mathbf{b}_2^* + \mathbf{b}_3^* \mathbf{c}_2^*, \quad \mathbf{c}_3^* \mathbf{b}_1^* + \mathbf{b}_3^* \mathbf{c}_1^*, \quad \mathbf{b}_3^*, \quad \mathbf{c}_2^* \mathbf{c}_1^* \mathbf{t}_3^* - \mathbf{c}_3^* \mathbf{c}_1^* \mathbf{t}_2^* + \mathbf{c}_3^* \mathbf{c}_2^* \mathbf{t}_1^*, \\
& \mathbf{c}_2^* \mathbf{t}_3^* - \mathbf{c}_3^* \mathbf{t}_2^*, \quad \mathbf{c}_1^* \mathbf{t}_3^* - \mathbf{c}_3^* \mathbf{t}_1^*, \quad \mathbf{t}_3^*, \quad \mathbf{c}_2^* \mathbf{b}_2^* \mathbf{c}_1^* + \mathbf{c}_3^* \mathbf{c}_1^* \mathbf{b}_1^*, \\
& \mathbf{c}_2^* \mathbf{b}_2^* - \mathbf{c}_3^* \mathbf{b}_1^*, \quad \mathbf{b}_2^* \mathbf{c}_1^*, \quad \mathbf{b}_2^*, \quad \mathbf{c}_2^* \mathbf{c}_1^* \mathbf{t}_2^* - \mathbf{c}_3^* \mathbf{c}_1^* \mathbf{t}_1^*, \quad \mathbf{c}_2^* \mathbf{t}_2^* - \mathbf{c}_3^* \mathbf{t}_1^*, \\
& \mathbf{c}_1^* \mathbf{t}_2^*, \quad \mathbf{t}_2^*, \quad \mathbf{c}_2^* \mathbf{c}_1^* \mathbf{b}_1^*, \quad \mathbf{c}_2^* \mathbf{b}_1^*, \quad \mathbf{c}_1^* \mathbf{b}_1^*, \quad \mathbf{b}_1^*, \\
& \mathbf{c}_2^* \mathbf{c}_1^* \mathbf{t}_1^*, \quad \mathbf{c}_2^* \mathbf{t}_1^*, \quad \mathbf{c}_1^* \mathbf{t}_1^*, \quad \mathbf{t}_1^*, \quad \mathbf{c}_3^* \mathbf{c}_2^* \mathbf{c}_1^*, \quad \mathbf{c}_3^* \mathbf{c}_2^*, \quad \mathbf{c}_3^* \mathbf{c}_1^*, \\
& \mathbf{c}_2^* \mathbf{c}_1^*, \quad \mathbf{c}_3^*, \quad \mathbf{c}_2^*, \quad \mathbf{c}_1^*, \quad 1.
\end{aligned}$$

We will provide the 256 elements for $n = 4$ in appendix A just to give an idea of how fast the expressions grow when we move to longer intervals.

The computation of the basis elements is much less time consuming compared to most other computations performed in this work. Since a printout of the elements would not make any sense, we shall only give an idea of the size of the expressions:

n	# Elements	Size of file
1	4	80 B
2	16	431 B
3	64	2,6 KiB
4	256	19 KiB
5	1024	161 KiB
6	4096	1,6 MiB
7	16384	18 MiB

Even though we can easily compute basis elements for even larger intervals, they are only useful for us if we can actually insert the explicit creation operators and carry out the necessary multiplications. Since this step requires much more computation time and memory, we refrain from going further.

There remains one problem associated with this last multiplication. Even though we know that all elements of the basis for an interval length of n are operators of at most length n , this does not necessarily apply to every single term which we need to compute: Consider as an example the element $\mathbf{c}_2^* \mathbf{b}_1^* + \mathbf{b}_2^* \mathbf{c}_1^*$ from the $n = 2$ basis. We know that $\ell(\mathbf{c}_2^* \mathbf{b}_1^* + \mathbf{b}_2^* \mathbf{c}_1^*) \leq 2$ but not that $\ell(\mathbf{c}_2^* \mathbf{b}_1^*) \leq 2$.

This means that we need to take the maximum possible length of every term into account. In the case of $n = 2$ this means that we have to use the creation operators constructed for an interval length of 3, which makes the computations much more involved. This simple issue makes the use of the JMS theorem very inefficient compared to using the exponential form of the density matrix.

We confirmed explicitly that it is possible to compute expectation values using the JMS theorem but for lengths greater than 3 this becomes very inefficient.

6.1.2 Change of Basis

In order to express a local operator in terms of the fermionic basis, it remains only to solve a linear system of equations. We shall provide some small examples in this section. Consider the operator $\sigma_1^z \sigma_n^z$. We will express it in terms of the basis for length n , but as explained before it will be necessary to use creation operators of greater lengths in the process.

$n = 2$

For the basis of length $n = 2$ the use of operators acting on an interval of length 3 is sufficient. To express an operator of length 2 it is therefore necessary to solve a system of 64 equations. As an example consider

$$\begin{aligned}
\sigma_1^z \sigma_2^z = & \\
& \frac{(q^2 + 1)^2 y^2}{4(y^2 - q^2)(q^2 y^2 - 1)} \cdot (\mathbf{t}_1^*)^2 + \frac{(q^2 - 1)^2 y (y^2 + 1)^2}{2(y^2 - 1)(y^2 - q^2)(q^2 y^2 - 1)} \cdot (\mathbf{c}_2^* \mathbf{b}_1^* + \mathbf{b}_2^* \mathbf{c}_1^*) \\
& + \frac{(q^4 - 1) y (y^2 + 1)}{2(q^4 y^2 - q^2 (y^4 + 1) + y^2)} \cdot \mathbf{c}_1^* \mathbf{b}_1^* + \frac{(q^2 + 1)^2 y (y^2 + 1)}{2(q^2 - y^2)(q^2 y^2 - 1)} \cdot \mathbf{t}_1^* \\
& - \frac{(q^2 + 1)^2 (y^2 + 1)^2}{4(q^2 - y^2)(q^2 y^2 - 1)} \cdot \mathbf{id} \quad (6.1)
\end{aligned}$$

and

$$\begin{aligned}
\sigma_1^x \sigma_2^x = & \\
& + \frac{q(q^2+1)y^2}{4(q^2-y^2)(q^2y^2-1)} \cdot (\mathbf{t}_1^*)^2 + \frac{(q^2-1)^2(q^2+1)y^3}{2q(y^2-1)(q^2-y^2)(q^2y^2-1)} \cdot (\mathbf{c}_2^* \mathbf{b}_1^* + \mathbf{b}_2^* \mathbf{c}_1^*) \\
& - \frac{(q^2-1)qy(y^2+1)}{2(q^2-y^2)(q^2y^2-1)} \cdot \mathbf{c}_1^* \mathbf{b}_1^* - \frac{q(q^2+1)y(y^2+1)}{2(q^2-y^2)(q^2y^2-1)} \cdot \mathbf{t}_1^* - \frac{y^2}{4q^3} \cdot \mathbf{b}_2^* \mathbf{b}_1^* \\
& - \frac{q^3}{4(q^2y^2-1)(q^6y^2-1)} \cdot \mathbf{c}_2^* \mathbf{c}_1^* + \frac{q(q^2+1)(y^2+1)^2}{4(q^2-y^2)(q^2y^2-1)} \cdot \mathbf{id} . \quad (6.2)
\end{aligned}$$

Note that $\sigma_1^x \sigma_2^x$ contains two terms with spin ± 2 , while $\sigma_1^z \sigma_2^z$ contains only terms of spin 0.

6.1.3 Expectation Values

Once an operator is expressed in the manner above, we can use the JMS theorem to compute expectation values. More precisely, we compute expectation values for the elements of the fermionic basis. To obtain the expectation value of an arbitrary operator expressed in terms of the fermionic basis, we only need to compute the linear combination of known values.

As an example we shall provide the expectation values for the $n = 2$ fermionic basis:

$$\begin{aligned}
\langle \mathbf{b}_2^* \mathbf{b}_1^* \rangle &= 0, & \langle \mathbf{b}_1^* \mathbf{t}_2^* - \mathbf{b}_2^* \mathbf{t}_1^* \rangle &= 0, & \langle \mathbf{b}_1^* \mathbf{t}_1^* \rangle &= 0, \\
\langle (\mathbf{t}_1^*)^2 \rangle &= 4 - 8\varphi\alpha\eta, & \langle \mathbf{c}_2^* \mathbf{b}_1^* + \mathbf{b}_2^* \mathbf{c}_1^* \rangle &= \tilde{\omega}'_x \alpha, \\
\langle \mathbf{b}_2^* \rangle &= 0, & \langle \mathbf{c}_1^* \mathbf{t}_2^* - \mathbf{c}_2^* \mathbf{t}_1^* \rangle &= 0, & \langle \mathbf{t}_2^* \rangle &= -\varphi_x \alpha \eta, \\
\langle \mathbf{c}_1^* \mathbf{b}_1^* \rangle &= -\tilde{\omega}, & \langle \mathbf{b}_1^* \rangle &= 0, & \langle \mathbf{c}_1^* \mathbf{t}_1^* \rangle &= 0, \\
\langle \mathbf{t}_1^* \rangle &= 2 - 2\varphi\alpha\eta, & \langle \mathbf{c}_2^* \mathbf{c}_1^* \rangle &= 0, & \langle \mathbf{c}_2^* \rangle &= 0, \\
\langle \mathbf{c}_1^* \rangle &= 0, & \langle \mathbf{id} \rangle &= 1 .
\end{aligned}$$

Being able to compute such expectation values, we can now calculate more general values.

$n = 2$

As an example we shall provide the correlation functions $\langle \sigma_1^z \sigma_2^z \rangle$, $\langle \sigma_1^x \sigma_2^x \rangle$ as well as the emptiness formation probability $P(n) = 2^{-n} \langle \prod_{j=1}^n (1 + \sigma_j^z) \rangle$.

$$\langle \sigma_1^z \sigma_2^z \rangle = \text{cth}(\eta) \tilde{\omega} + \frac{\tilde{\omega}'_x}{\eta} \quad (6.3)$$

$$\langle \sigma_1^x \sigma_2^x \rangle = -\frac{\tilde{\omega}}{2\text{sh}(\eta)} - \frac{\text{ch}(\eta) \tilde{\omega}'_x}{2\eta} \quad (6.4)$$

$$P(2) = \frac{1}{4} - \frac{\varphi}{2} + \frac{\text{cth}(\eta) \tilde{\omega}}{4} + \frac{\tilde{\omega}'_x}{4\eta} . \quad (6.5)$$

The obtained correlation functions $\langle \sigma_1^z \sigma_2^z \rangle$ and $\langle \sigma_1^x \sigma_2^x \rangle$ are the same as in [53]. The emptiness formation probability $P(2)$ differs from the paper in the last term, which is due to a typo in the paper. This can be verified by taking the density matrix $D_2(T, h)$ from [57] (which was cited in [53]) and simply evaluating

$$P(2) = \frac{1}{4} \text{tr}_{12} (D_2(T, h)(1 + \sigma_1^z)(1 + \sigma_2^z)) \quad (6.6)$$

by hand.

$n = 3$

As explained before, the computational effort needed to calculate expectation values using the JMS theorem grows rapidly because it is necessary to use operators acting on large intervals. Considering $n = 3$, the fermionic basis already contains elements like

$$\mathbf{b}_2^* \mathbf{b}_1^* \mathbf{t}_3^* - \mathbf{b}_3^* \mathbf{b}_1^* \mathbf{t}_2^* + \mathbf{b}_3^* \mathbf{b}_2^* \mathbf{t}_1^* .$$

Generally, to explicitly compute this basis element, we would need to use operators of length 6. Since the main computational effort lies in constructing the creation operators and multiplying them to obtain the basis elements, it becomes clear that the strategy explained in this section is not suitable for large intervals.

However, we do not know the actual length of the products above. Because of this we tried to construct the fermionic basis for $n = 3$ using operators only of length 4. Having constructed these elements we were able to show, that they indeed form a basis of the length 3 subspace. This fact motivated us to go further and try to obtain $\langle \sigma_1^z \sigma_3^z \rangle$ and $\langle \sigma_1^x \sigma_3^x \rangle$ and $P(3)$ using this basis. The resulting functions

$$\langle \sigma_1^z \sigma_3^z \rangle = 2 \text{cth}(2\eta) \tilde{\omega} + \frac{\tilde{\omega}'_x}{\eta} + \frac{\text{th}(\eta)(\tilde{\omega}_{xx} - 2\tilde{\omega}_{xy})}{4} - \frac{\text{sh}^2(\eta) \tilde{\omega}'_{xy}}{4\eta} \quad (6.7)$$

$$\langle \sigma_1^x \sigma_3^x \rangle = -\frac{\tilde{\omega}}{\text{sh}(2\eta)} - \frac{\text{ch}(2\eta) \tilde{\omega}'_x}{2\eta} - \frac{\text{ch}(2\eta) \text{th}(\eta)(\tilde{\omega}_{xx} - 2\tilde{\omega}_{xy})}{8} + \frac{\text{sh}^2(\eta) \tilde{\omega}'_{xy}}{8\eta} \quad (6.8)$$

are, remarkably, the same as in [53]. Even the emptiness formation probability can be obtained using only $n = 4$ operators, even though it is more complicated than the correlation functions, since it has no definite spin

symmetry:

$$\begin{aligned}
P(3) = & \frac{1}{8} - \frac{3\varphi}{8} + \frac{(q^4 + q^2 + 1)\tilde{\omega}}{2(q^4 - 1)} + \frac{(q^2 - 1)(\tilde{\omega}_{xx} - 2\tilde{\omega}_{xy})}{32(q^2 + 1)} \\
& + \frac{3(q^2 + 1)(-\varphi_{xx}\tilde{\omega} + 2\varphi_x\tilde{\omega}_x - 2\varphi\tilde{\omega}_{xy} + \varphi\tilde{\omega}_{xx})}{32(q^2 - 1)} + \frac{3\tilde{\omega}'_x}{8\eta} \\
& - \frac{(q^2 - 1)^2\tilde{\omega}'_{xxy}}{128\eta q^2} + \frac{(q^4 + 10q^2 + 1)(-\varphi_{xx}\tilde{\omega}'_x + \varphi_x\tilde{\omega}'_{xx} - \varphi\tilde{\omega}'_{xxy})}{128\eta q^2}. \quad (6.9)
\end{aligned}$$

This is, again, identical to the results of [53].

We refrain from using this approach for longer chains, as the essential results are already visible at this point. The calculation of arbitrary expectation values using the fermionic basis and the JMS theorem was implemented successfully. As explained before it seems that this approach is not ideally suited for the computer. It is however noteworthy, that there is obviously room for improvement using this approach. If it were possible to exactly obtain the actual length of all single terms in the fermionic basis one could choose the length of the involved operators optimally. For longer chains we shall use the exponential form of the density matrix.

6.2 Exponential Form

As mentioned before, using the JMS theorem to calculate expectation values presents the problem that we have to choose rather long intervals for the construction of the fermionic operators. This problem does not arise when using the exponential form of the density matrix due to the usage of annihilation operators. Because of this we can calculate expectation values on longer intervals using this approach.

The first objects which we computed using this approach were the correlation functions presented above for $n = 2, 3$ to provide a comparison and build confidence in our programs. In the next step we calculated $P(2)$ and $P(3)$ for the case of a vanishing external field and compared the results to the expressions presented above. As explained before in section 4.2 the function φ vanishes in this case. As expected we were able to reproduce the results of [53]:

$$P(2) = \frac{1}{4} + \frac{\text{cth}(\eta)\tilde{\omega}}{4} + \frac{\tilde{\omega}'_x}{4\eta}. \quad (6.10)$$

$$\begin{aligned}
P(3) = & \frac{1}{8} + \frac{(q^4 + q^2 + 1)\tilde{\omega}}{2(q^4 - 1)} + \frac{(q^2 - 1)(\tilde{\omega}_{xx} - 2\tilde{\omega}_{xy})}{32(q^2 + 1)} \\
& + \frac{3\tilde{\omega}'_x}{8\eta} - \frac{(q^2 - 1)^2\tilde{\omega}'_{xxy}}{128\eta q^2}. \quad (6.11)
\end{aligned}$$

After these basic checks we then went on to calculate the xx - and zz -correlators for $n = 4, 5$. For the case $n = 4$ these functions are known from [53] and are reproduced by our program. The correlation functions $\langle \sigma_1^z \sigma_5^z \rangle$ and $\langle \sigma_1^x \sigma_5^x \rangle$ are printed out in appendix B due to their size.

6.2.1 Comparison with Kato et al.

We also compared our results to the work of Kato et al. in [63, 64]. The authors show that the known multiple integral representations of correlation functions can be reduced to one-dimensional integrals in the ground state. These integrals are then solved analytically for the case that Δ is equal to certain roots of unity. The correlations $\langle \sigma_1^z \sigma_n^z \rangle$ and $\langle \sigma_1^x \sigma_n^x \rangle$ are given exactly for $n = 2, 3, 4$ and $\eta = 0, \frac{i\pi}{2}, \frac{i\pi}{3}, \frac{i\pi}{4}, \frac{i\pi}{5}, \frac{i\pi}{6}, \frac{i2\pi}{3}, \frac{i3\pi}{4}, i\pi$. In the ground state the functions \mathfrak{b} and $\bar{\mathfrak{b}}$ given in [53] become zero which greatly simplifies the calculation of the functions ω and ω' . Because of this it is easy to compute these functions using Mathematica. Since we did not cover the case of q being a root of unity, we compute all correlation functions for values slightly above and below the given values of η and interpolate. Numerical problems are generally expected, since expectation values may have poles if q is a root of unity. The functions given above for $n = 2, 3$ obviously have a pole only at $\eta = 0$, but starting with $n = 4$ more poles appear. These poles are removed by the behaviour of the functions ω and ω' : At these points their real parts vanish and their imaginary parts cancel each other out. As is to be expected, the numerical problem becomes more severe for bigger values of n . In this approach it is not surprising, that the quality of the results depends on the chosen shift in a non-trivial manner. As expected, the differences to Katos results will become smaller with smaller shifts, but below some point numerical problems arise. For the majority of the results the relative differences to the given values will become small ($< 10^{-6}$) in this approach, which we take as a reasonably good agreement with [63, 64]. There are two exceptions: On the one hand some values are predicted to be zero. In these cases we cannot sensibly calculate the relative difference, but the resulting absolute values are reasonably small (also $< 10^{-6}$). On the other hand the points $\eta = 0$ and $\eta = i\pi$, i.e. $\Delta = 1$ and $\Delta = -1$, are very difficult to handle, the first case more so than the second. For these cases it makes no sense to evaluate values on both sides, since the definition of ω from [53] is only valid for the massless regime, i.e. $|\Delta| < 1$. For this reason we try to take the limits one-sided in these cases. If the shifts are chosen too small, the resulting values will diverge due to numerical problems. Despite these problems, we can control the relative errors at these points to be smaller than 0.01. In conclusion we are certain that our results are in accordance to [63, 64].

After the comparison with previous works we are reasonably certain that our programs produce correct results for arbitrary interval lengths. This is confirmed by various tests we applied to different objects. Our experience is

that even a small error in one of the programs will lead to completely wrong results. It may sometimes happen, that an existing error does not manifest itself for an interval length of $n = 2$. But in our experience potential errors occur very reliably for interval lengths of $n \geq 3$.

6.2.2 Comparison with Lukyanov and Terras

We shall do a last comparison of our results with a previous work, even though we are quite confident in our results at this point. Lukyanov and Terras consider the long-distance asymptotic behaviour of the correlation functions $\langle \sigma_1^x \sigma_n^x \rangle$ and $\langle \sigma_1^z \sigma_n^z \rangle$ in their works [65, 66], using Gaussian conformal field theory. A comparison with these asymptotics will not only be an additional test for our results for $T = h = 0$. Rather, it will be interesting to see at which distance the asymptotic expressions become good approximations of the correlation functions. They obtain

$$\begin{aligned} \langle \sigma_1^x \sigma_n^x \rangle \sim & \frac{(-1)^n A}{n^\nu} \left\{ 1 - \frac{B}{n^{4/\nu-4}} + \mathcal{O}\left(n^{-2} \log n, n^{8-8/\nu}\right) \right\} \\ & - \frac{\tilde{A}}{n^{\nu+1/\nu}} \left\{ 1 + \frac{\tilde{B}}{n^{2/\nu-2}} + \mathcal{O}\left(n^{-2} \log n, n^{4-4/\nu}\right) \right\} + \dots \end{aligned} \quad (6.12)$$

and

$$\begin{aligned} \langle \sigma_1^z \sigma_n^z \rangle \sim & -\frac{1}{\pi^2 \nu n^2} \left\{ 1 + \frac{\tilde{B}_z}{n^{4/\nu-4}} \left(1 + \frac{2-\nu}{2(1-\nu)} \right) + \mathcal{O}\left(n^{-2} \log n, n^{8-8/\nu}\right) \right\} \\ & + \frac{(-1)^n A_z}{n^{1/\nu}} \left\{ 1 - \frac{B_z}{n^{2/\nu-2}} + \mathcal{O}\left(n^{-2} \log n, n^{4-4/\nu}\right) \right\} + \dots \end{aligned} \quad (6.13)$$

where $A, B, \tilde{A}, \tilde{B}, A_z, B_z, \tilde{B}_z$ are functions depending only on ν which are given in their work. In this context ν is given by $\Delta = \cos(\pi(1-\nu))$. The reason for this choice is that [65, 66] do not use the same Hamiltonian as we do, but instead

$$H_{XXZ} = -\frac{J}{2} \sum_{k=-\infty}^{\infty} (\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta (\sigma_k^z \sigma_{k+1}^z - 1)) , \quad J > 0 .$$

This choice is however unitary equivalent to ours, as the substitutions $J \rightarrow -J$ and $\Delta \rightarrow -\Delta$ are equivalent to the unitary transformation $H \rightarrow U H U$ with $U = \prod_{j=-\infty}^{\infty} \sigma_{2j}^z$. Therefore we can consider their choice to be equivalent to ours with the above choice for Δ . To compare our results to the given asymptotics, we introduced an additional factor $(-1)^n$ to $\langle \sigma_1^x \sigma_n^x \rangle$ as opposed to the original expressions, the reason being the transformation U .

To make a comparison to our results, we take the definition of the function ω from [53]. For $T = h = 0$ the auxiliary functions \mathfrak{b} and $\bar{\mathfrak{b}}$ given in this paper

vanish. This makes the calculation of the functions ω and ω' much easier, since only simple integrals remain. These can then be solved numerically using Mathematica.

Considering the above expressions, we see that the order in which we have to observe the terms depends on ν . For the sake of simplicity, we shall only distinguish between different terms of the expressions if they can be ordered for general $0 < \nu < 1$. For this reason we shall consider two approximations in the case of $\langle \sigma_1^x \sigma_n^x \rangle$: on the one hand we shall consider only the first term $\frac{A}{n^\nu}$, which is the leading term for general ν , and on the other hand we consider the whole expression. In the case of $\langle \sigma_1^z \sigma_n^z \rangle$ we shall only consider the whole expression. The reason is that only the term containing \tilde{B}_z can be shown to be of higher order than the rest. However, it makes no visible difference whether we include it in our plots or not.

Looking at the figures 6.1 and 6.2 showing $\langle \sigma_1^z \sigma_n^z \rangle$ and $\langle \sigma_1^x \sigma_n^x \rangle$ respectively, we observe that there are poles in the asymptotic expansion. For $\Delta \rightarrow -1$, i.e. $\nu \rightarrow 0$ there are rapid oscillations in all plots, becoming less prominent for increasing n . These oscillations are no numerical error but rather a feature of the functions $B, \tilde{B}, B_z, \tilde{B}_z$. The visible poles in $\langle \sigma_1^x \sigma_n^x \rangle$ stem from the function B , which has poles of order 2 at $\nu = \frac{2}{3+2l}$ for $l \in \mathbb{N}$. At these positions q is a root of unity. As can be seen in the plots, the poles become narrower with increasing n .

Aside from roots of unity, we observe the expected behaviour: For the nearest neighbour functions the asymptotic expansion differs greatly from the exact results. The agreement between the results becomes better with increasing n . It is noteworthy, that the asymptotics agree very well with the exact values even for short distances. Especially for the xx two-point functions the results agree very well.

We take this as a successful plausibility check for our results for $n = 5$.

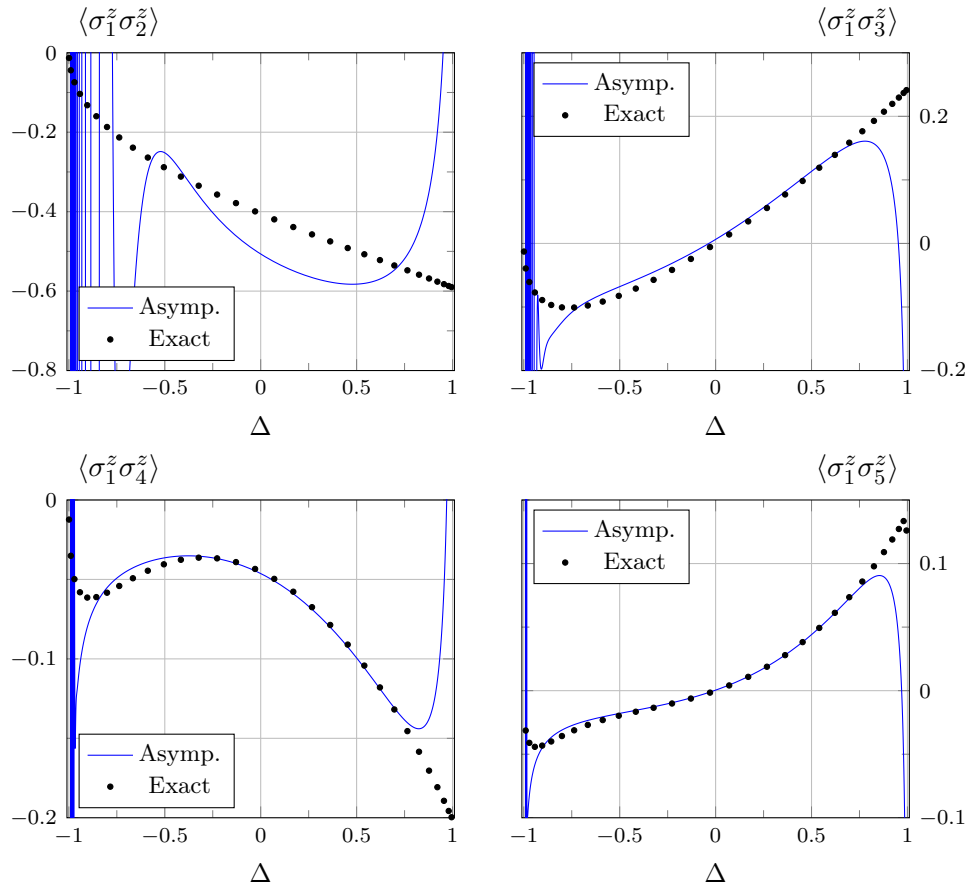


Figure 6.1: Two-point correlators $\langle \sigma_1^z \sigma_n^z \rangle$ for $n = 2, 3, 4, 5$ in the ground state and at zero magnetic field in the massless regime.

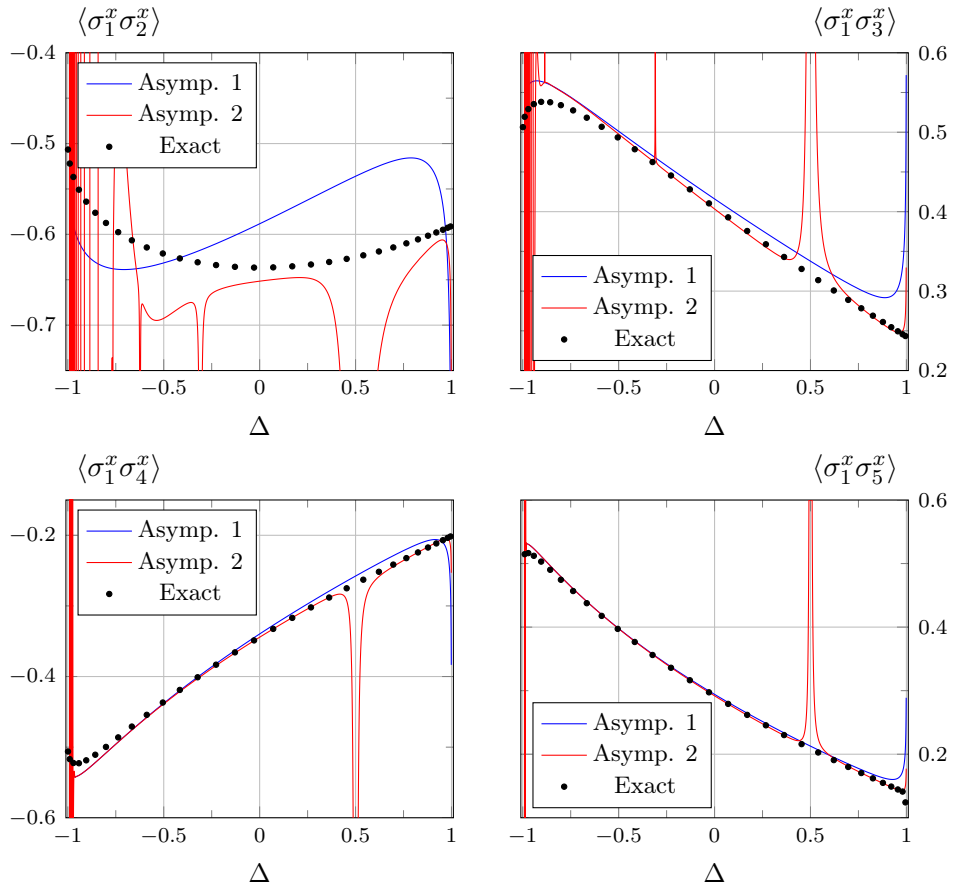


Figure 6.2: Two-point correlators $\langle \sigma_1^x \sigma_n^x \rangle$ for $n = 2, 3, 4, 5$ in the ground state and at zero magnetic field in the massless regime.

6.3 Correlation Functions

In this section we will present plots of the correlation functions presented above as functions of T and h for different values of the other parameters. For this purpose we will use the functions presented above and in appendix B. The function ω , as well as its derivatives, are calculated using the program mentioned in section 5.13.

We use the same choices of parameters as in [53] to compare our work to the paper and to extend this work to $n = 5$. The only difference is our choice of $\Delta = 0.707$ instead of $\Delta = 1/\sqrt{2}$. We make this change because in the case $\Delta = 1/\sqrt{2}$ we have $\eta = \frac{i\pi}{4}$ which means that q is a root of unity.

Coincidentally, for $n = 2, 3, 4$ there are no poles in $\langle \sigma_1^z \sigma_n^z \rangle$ or $\langle \sigma_1^x \sigma_n^x \rangle$ at the point $\eta = \frac{i\pi}{4}$, which is why there was no problem in the paper with this particular choice. However, moving to $n = 5$ makes poles appear at this point. To get an idea of the poles appearing in the correlation functions we shall give a short overview in table 6.1.

Table 6.1: Values of $\gamma = -i\eta$ at which the correlation functions have poles.

n	$\langle \sigma_1^z \sigma_n^z \rangle$	$\langle \sigma_1^x \sigma_n^x \rangle$
2	πk	πk
3	$\pi \frac{k}{2}$	$\pi \frac{k}{2}$
4	$\pi \frac{k}{3}, \pi \frac{2k+1}{2}$	$\pi \frac{k}{3}$
5	$\pi \frac{k}{3}, \pi \frac{k}{4}$	$\pi \frac{k}{3}, \pi \frac{k}{4}$

The first few correlation functions for $n = 2, 3, 4$ are shown in figures 6.3 and 6.4 depending on T . As expected these plots look like the ones given in [53]. Here we can observe the expected behaviour: The transversal functions alternate their signs with n , as do the longitudinal functions for $\Delta > 0$. Of course the alternating behaviour of the longitudinal functions changes with sufficiently large external field h . For very large h the system enters the ferromagnetic phase so the longitudinal correlations become equal to one and the transversal correlations vanish for low temperatures. In the case of negative Δ the longitudinal correlations are always negative for low T and change to positive at some ‘‘crossover temperature’’. This effect is known as ‘‘quantum-classical crossover’’ and was studied in [67–69]. We will compare the crossover temperatures obtained from our results with [67], where the crossover was studied numerically, later in subsection 6.3.1. Of course all correlations vanish for sufficiently large temperatures.

The curves presented showcase a competition between three influences: first the external field which aligns the spins in z direction. Second the longitudinal exchange coupling which tends to produce an antiparallel (parallel)

spin alignment for $\Delta > 0$ ($\Delta < 0$). Third the transversal exchange coupling which can be interpreted as a kinetic term of the Hamiltonian or quantum fluctuation. Figures 6.3 and 6.4 suggest that the relative strength of these effects varies with temperature. At low temperatures the quantum fluctuations seem to have a dominant influence, reducing the correlations from ± 1 . At higher temperatures the influence of the fluctuations seems to weaken, as the spins become aligned by the magnetic field or the longitudinal coupling in the case $\Delta < 0$. The absence of this effect for $\Delta > 0$ might be explained by the influence of the rising temperature contesting the longitudinal coupling.

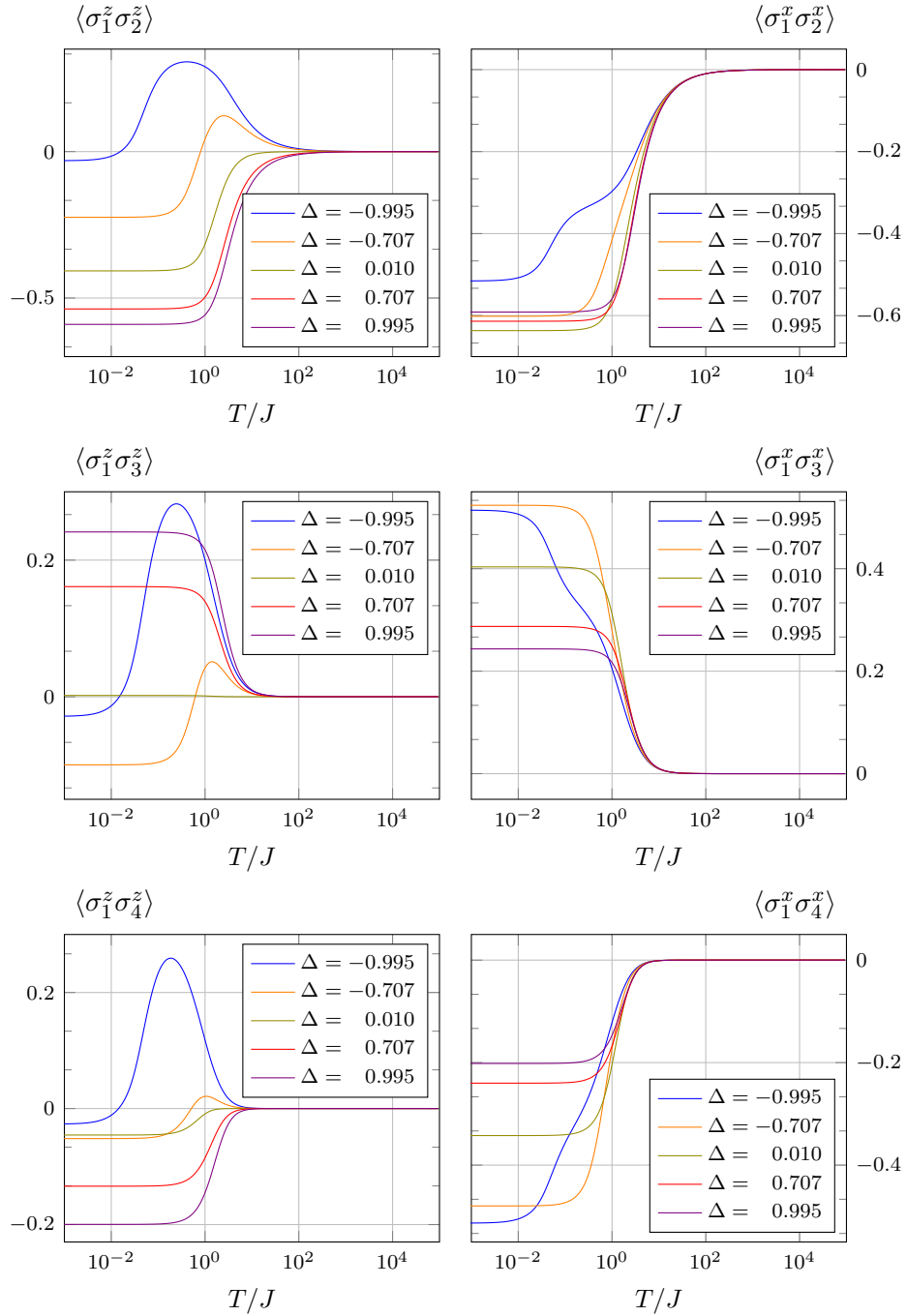


Figure 6.3: Two-point correlation functions for $n=2,3,4$ for different values of Δ at $h = 0$ in the critical phase.

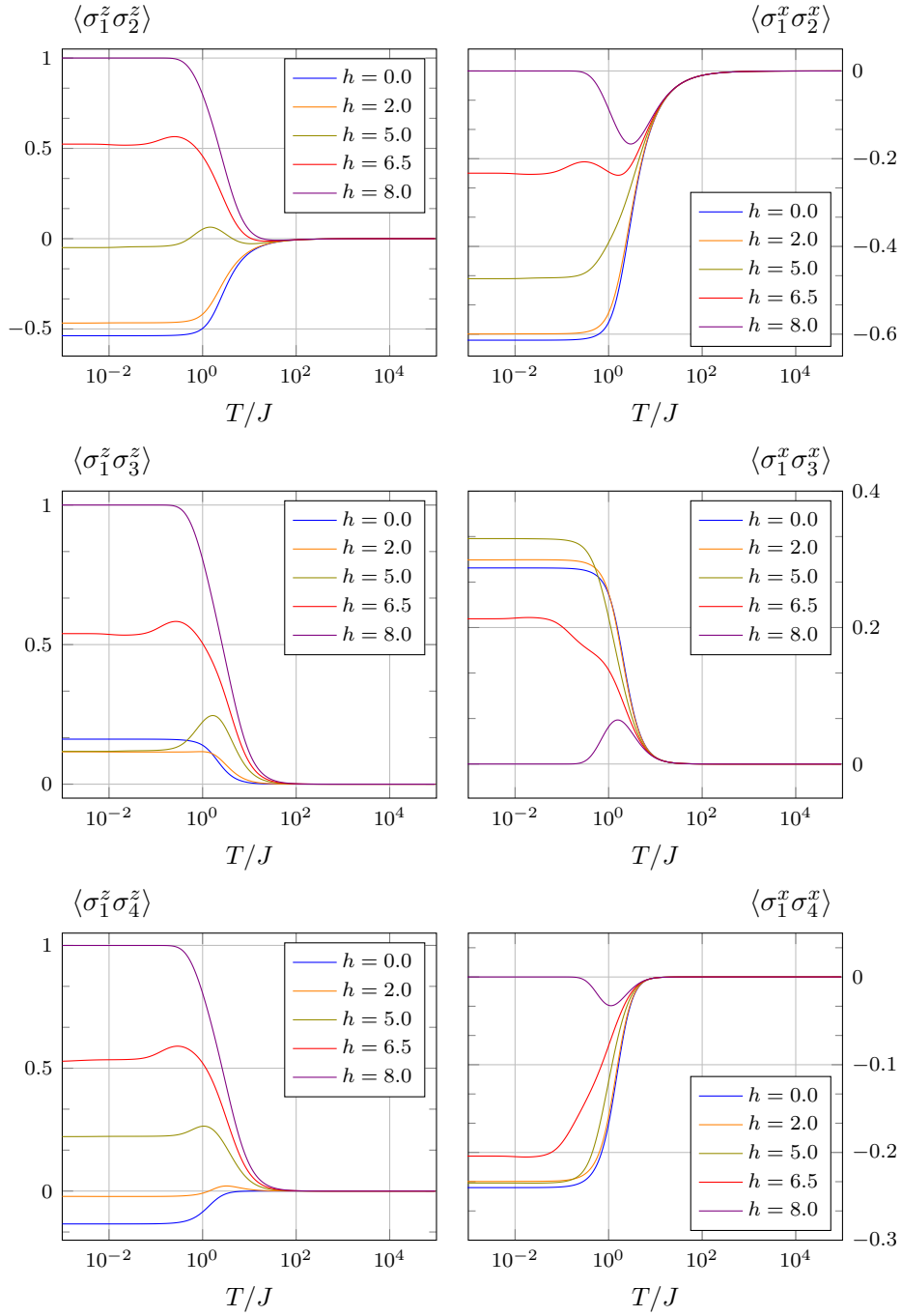


Figure 6.4: Two-point correlation functions for $n=2,3,4$ for different values of h at $\Delta = 0.707$ in the critical phase.

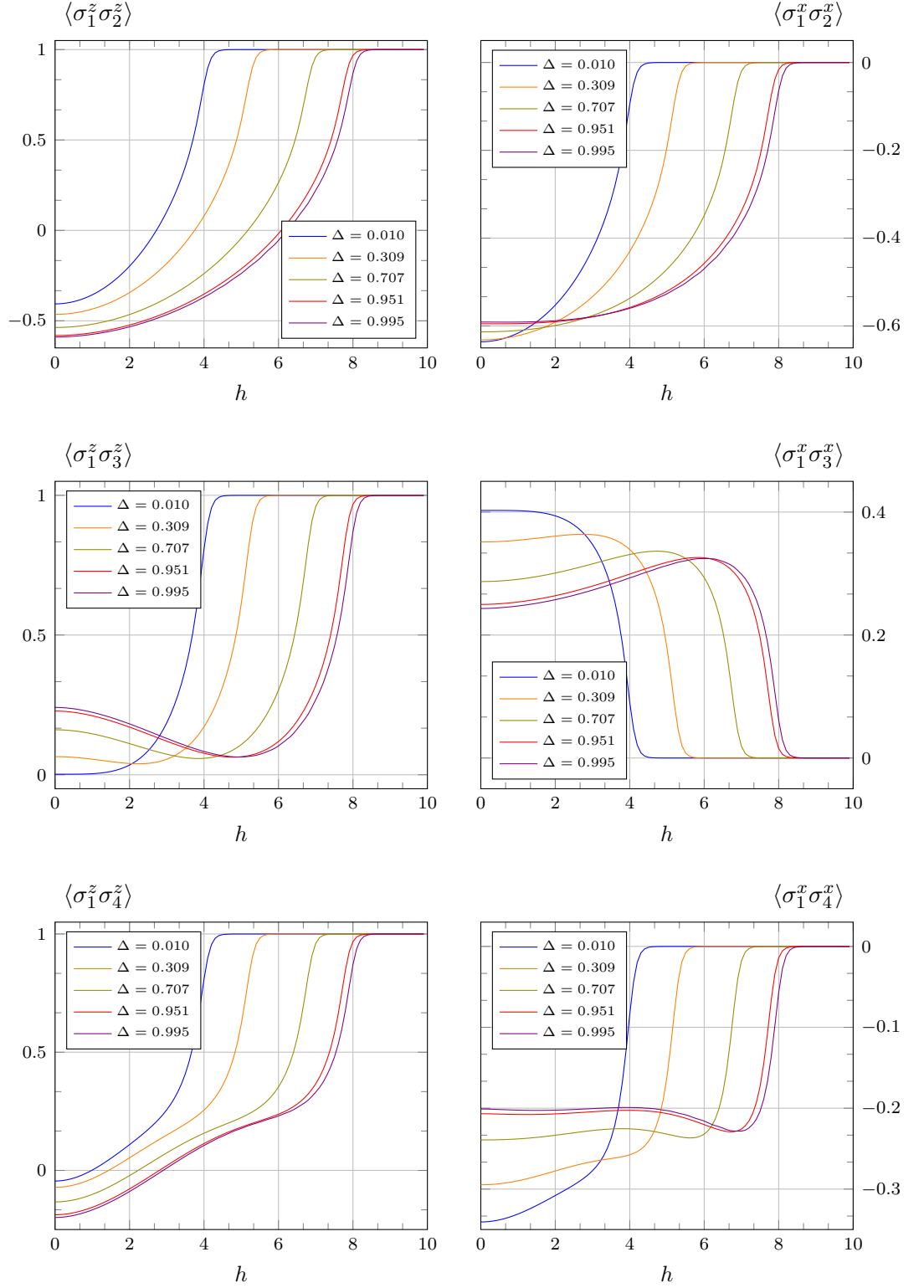


Figure 6.5: Two-point correlation functions for $n=2,3,4$ for different values of Δ at $T/J = 0.1$ in the critical phase.

Figure 6.5 shows the correlation functions for varying external field h for up to $n = 4$. As before, we can observe the expected behaviour. For low enough h and positive Δ the signs of the correlations alternate with n . Increasing h aligns all spins so that the longitudinal correlations tend to one and the transversal ones tend to zero, eventually reaching saturation at the upper critical field $h_u = 4J(\Delta + 1)$ shown in the phase diagram. The points at which saturation is reached will become more sharply distinguished if the temperature is decreased and will be smoothed out if T increases. An interesting feature is that the correlations may depend non-monotonically on h for intermediate fields.

Additionally we can see a clear difference to the results presented in [53] for $n = 4$ and $\Delta = 0.995$. We strongly believe that our results are the correct ones in this case. The reason is simply the choice of integration parameters passed to the program: the plots in figure 6.5 were made with 2^{22} discretization points and a cut-off of $C = 8000$. We can roughly reproduce the plots shown in [53] if we choose 2^{17} points and $C = 250$. Note that, with this smaller choice of parameters, the plots change depending on the convention used for the derivatives. In the paper the y -convention is used. To reproduce these plots we chose the same convention. However, using the lower choice for the integration parameters, the plots will change if we shift to the x -convention which should obviously not be the case. Figure 6.6 shows

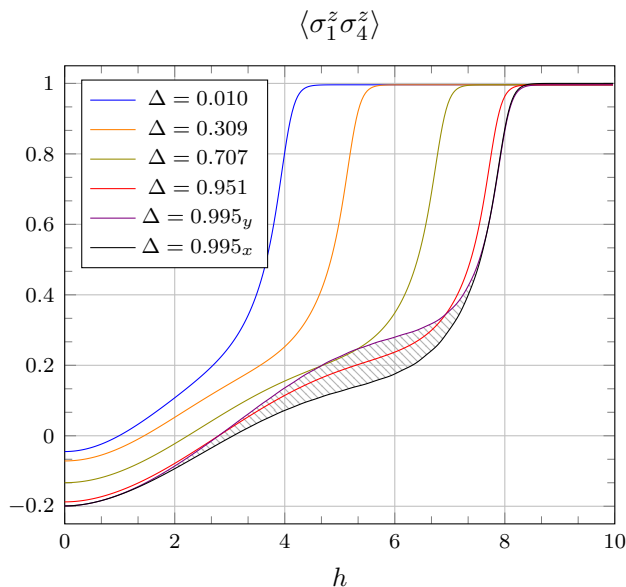


Figure 6.6: Correlations for variable h and $T/J = 0.1$. The purple and black curves are for the y - and x -convention. The difference has been shaded. For all other curves both conventions coincide. Integration parameters are 2^{17} points and $C = 250$.

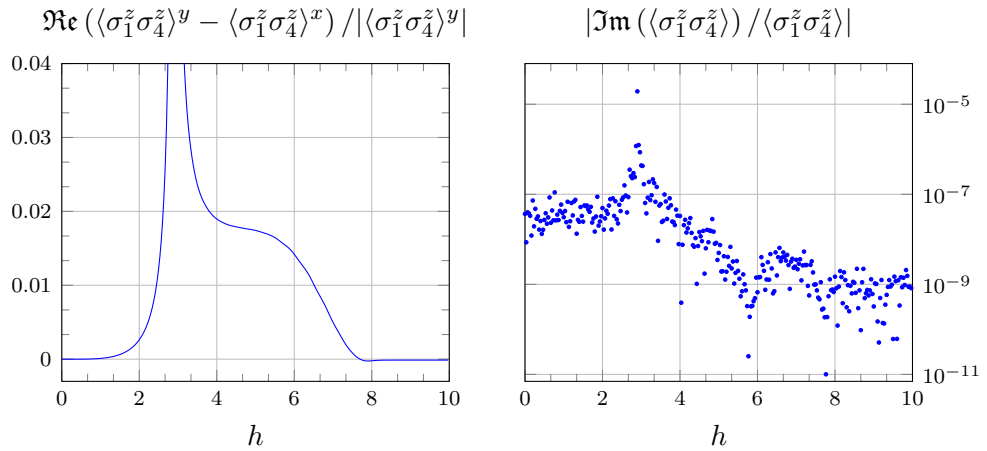


Figure 6.7: Left: Real part of the relative differences between the x - and y -conventions. A superscript x/y indicates the x/y -convention. The pole appears due to the correlation function being zero at this point. Right: The imaginary part. Each point shows the maximal imaginary part between both conventions for the derivatives of ω . Both for $T/J = 0.1$ and $\Delta = 0.995$.

this difference. By increasing the settings for the numerical integration the difference area shown shrinks until both curves finally coincide. Using our higher choice of parameters the curves for both conventions coincide nearly perfectly. Figure 6.7 shows the relative difference between those two curves using our choice of the integration parameters as well as the corresponding imaginary part. It is clear that both error measures are reasonably small in our case. The pole in the relative difference between both conventions is due to the correlation function being zero at this position.

Moving on to the case $n = 5$ it is clear that we have even higher requirements for the numerical precision of ω than before. This becomes apparent when we insert the values for ω that we used until now. The curve for variable h and $\Delta = 0.995$, which was problematic for $n = 4$, becomes unmanageable in the case $n = 5$. This is immediately obvious since we obtain correlation functions with real and imaginary parts whose absolute values are greater than 1000. As we explained before, the difference functions $\omega_{ij}^{(l)}$ are a measure for a specific type of numerical error which was dominant for the cases $n \leq 4$. For $n = 5$ it seems that other errors become dominant which can likely be explained by the sheer complexity of the rational functions for the correlation functions. One very simple criterion for the quality of the results is their imaginary part. Obviously, it should be zero for all correlation functions, but as mentioned above it becomes very large for the most problematic case. For all functions shown so far ($n \leq 4$) the absolute values of the imaginary parts of the correlation functions are smaller than 10^{-7} , which we believe to be

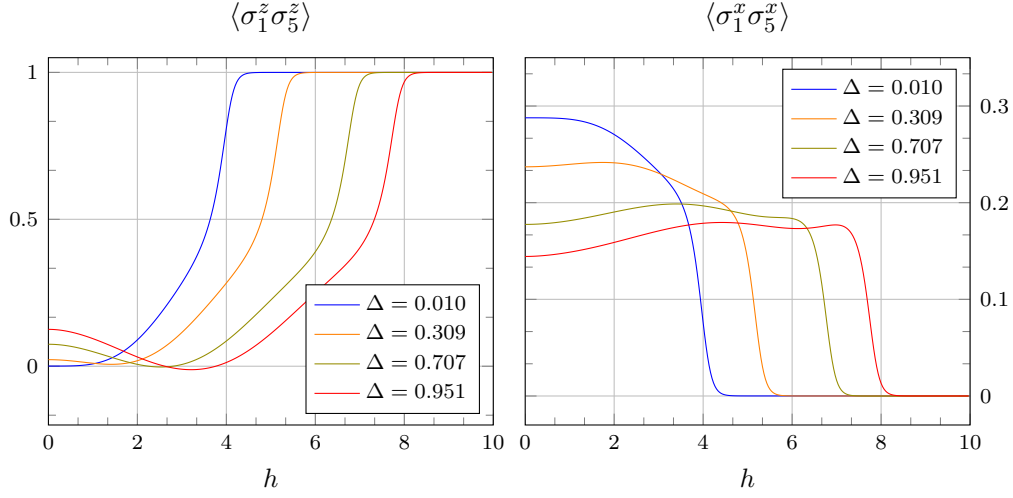


Figure 6.8: Two-point functions for $n = 5$ and $T/J = 0.1$.

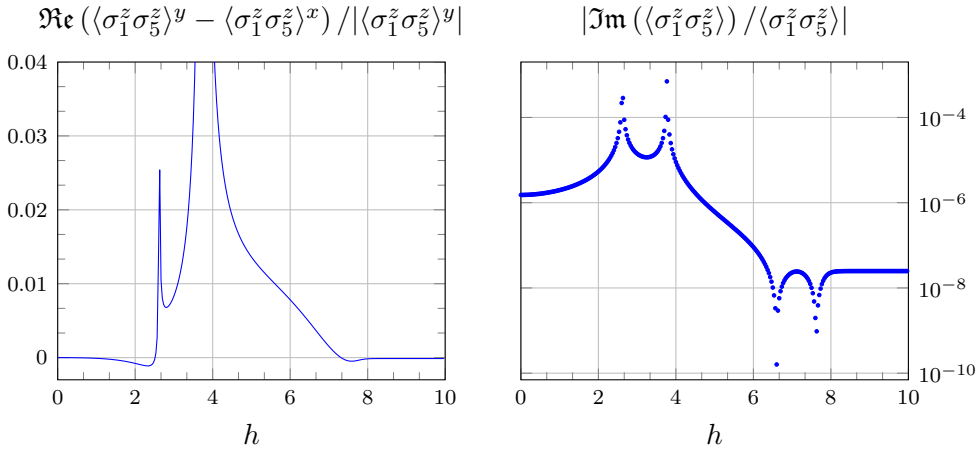


Figure 6.9: Left: Relative difference between the real parts for both conventions. Right: The imaginary part. Both for $\Delta = 0.951$ and $T/J = 0.1$. The poles appear again due to zeros in the correlation function.

reasonable. For $n = 5$ we consider these imaginary parts as an additional criterion for the quality of the results.

As first example of $n = 5$ two-point functions we consider the case of variable field h which is shown in figure 6.8. The case $\Delta = 0.995$ is left out because of the numeric problems mentioned earlier. We will provide error plots for this case later. First we want to build some trust in the results which are shown. As expected, the numerical difficulties become greater with larger Δ , which is why we will examine the difference function and imaginary part for $\Delta = 0.951$, as this is the largest value used in the plot.

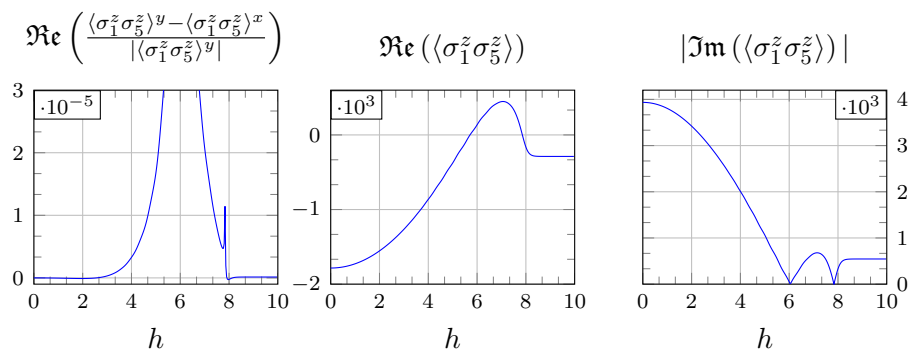


Figure 6.10: From left to right: Relative difference between the real parts for both conventions, the real part and the imaginary part for $\Delta = 0.995$ and $T/J = 0.1$.

These are presented in figure 6.9. As before with $n = 4$, both error measures are reasonably small even in the case $n = 5$ and $\Delta = 0.951$. Next, we want to show an example for unusable results which have to be rejected due to numerical errors. Figure 6.10 shows the same quantities as above as well as the real part for the case $\Delta = 0.995$, which we have spared out in figure 6.8. It is immediately apparent that these results cannot be correct even though the difference function seems to indicate a small error. This shows that we cannot rely on a single criterion to gauge the numerical accuracy of our results.

At this point it is clear that we can detect numerical errors in the function ω well enough to be confident in our results. Most of the time errors can be controlled by setting the right parameters for the integration. The case of $n = 5$ and $\Delta = 0.995$ is the only case which we encountered so far where this is not possible. Considering how close this case is to the point $\Delta = 1$ the difficulties are not surprising. We believe that it would be possible to obtain results for this case by improving the program responsible for calculating ω . However, the time necessary would likely not be justified by the limited results.

At last we show the correlation functions in dependence of the temperature T in figure 6.11 and figure 6.12. The same considerations described above were made concerning the numerical errors but for the sake of brevity these will not be shown here. The errors of all presented results are reasonably small.

It should be noted that all results for $n = 5$ exhibit the expected behaviour which was already described above.

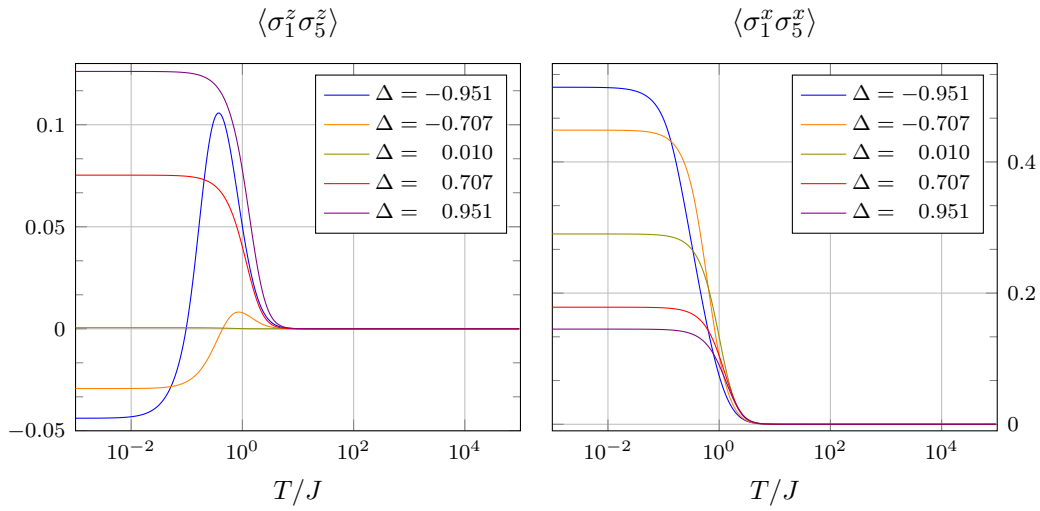


Figure 6.11: Two-point functions for $n = 5$ and $h = 0$.

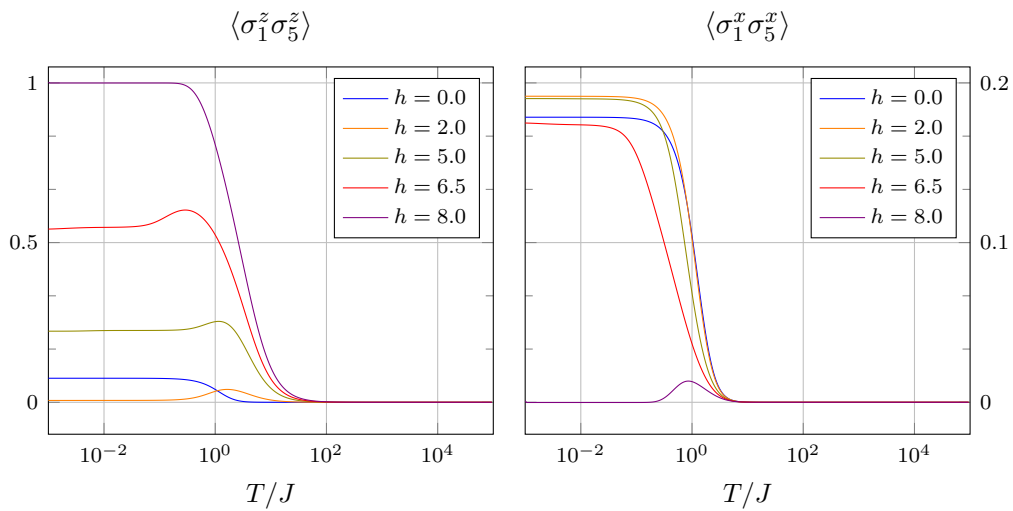


Figure 6.12: Two-point functions for $n = 5$ and $\Delta = 0.707$.

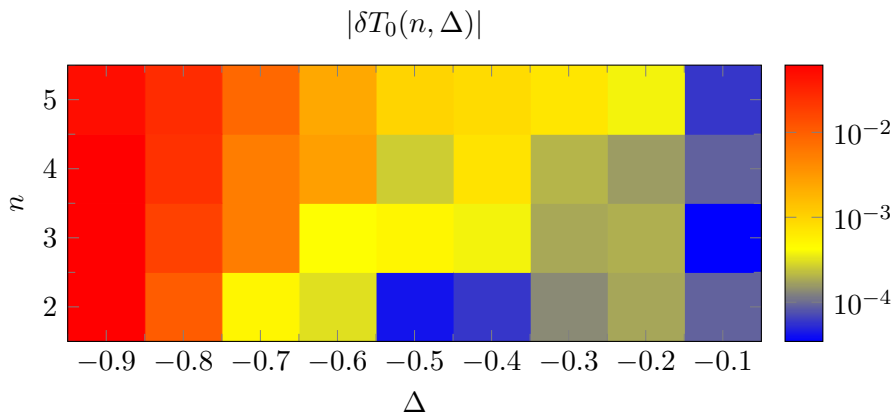


Figure 6.13: Relative differences between crossover temperatures obtained from our results and [67].

6.3.1 Crossover Temperatures

In this section we will compute the crossover temperatures at which the longitudinal correlations $\langle \sigma_1^z \sigma_n^z \rangle$ change their sign from negative to positive for $-1 < \Delta < 0$ and $h = 0$. After that we will compare these temperatures to the ones obtained in [67]. We do not expect an exact agreement between our results and [67], as their results are obtained using a numerical diagonalization for a finite chain of $N = 18$ sites. Because of finite-size effects we expect that, in general, differences will grow with increasing n . However, it is not known in advance at which value of n these effects will become significant. Additionally, we expect some “noise” due to numerical inaccuracies.

Having already calculated the functions $\langle \sigma_1^z \sigma_n^z \rangle$ it is easy to obtain the crossover temperatures $T_0(n, \Delta)$, as these are simply the roots of the correlations. However, since the correlation functions are not known as a closed expression but instead as a list of points, we cannot rely on predefined features of e.g. Mathematica to find their roots. Instead, we search the lists of points from left to right for the first neighbouring points with different signs. We then interpolate between these points to find the crossover temperatures. Interpolation is done using polynomials of different degrees. Starting from the two identified points, we add the nearest $2k$ points on both sides to obtain polynomials of degree $2k + 1$. We tested the procedure for degrees 1, 3 and 5, measuring the relative change between these steps. Even for the step from degree 1 to 3, over all obtained temperatures, the biggest relative change was smaller than one percent, meaning that the choice of the degree only makes a negligible difference. We then used a polynomial of 5th degree for the final values since we had already prepared the needed code.

All obtained temperatures, as well as the corresponding values from [67]

are shown in appendix C. The relative differences

$$\delta T_0(n, \Delta) = \frac{T_0(n, \Delta) - \tilde{T}_0(n, \Delta)}{T_0(n, \Delta)}, \quad (6.14)$$

where $T_0(n, \Delta)$ are the temperatures obtained from our results and $\tilde{T}_0(n, \Delta)$ are the ones from [67], are shown in figure 6.13 as a heatmap. The biggest differences can be observed for $\Delta = -0.9$ and have values around 6%. However, the majority of the values lies well below 1%. The figure shows that, in general, the differences grow with increasing n , as expected.

Along the Δ -axis we observe increasing deviations as Δ moves towards -1 . One possible explanation for this might be our own numerical precision. As mentioned before, this precision is limited by the computation of ω and its derivatives. However, at $h = 0$ and $|\Delta| \leq 0.9$ we do not expect big numerical uncertainties in our calculations. To test our own precision we enlarged the integration parameters for ω and verified that the $\delta T_0(n, \Delta)$ changed very little. This suggests that the explanation for the differences lies in [67]. There is little ground to assess the numerical precision of the paper or the influence of finite-size effects. Regarding the finite-size effects however, the authors included data for the correlation functions at $\Delta = -0.9$ for chain lengths of $N = 16$ and $N = 18$ in tables 3 and 5. We did a simple comparison of the provided correlation functions for the two different chain lengths at $T = 0.1$, which is close to the crossover temperatures at $\Delta = -0.9$. The differences between these values range from 3% to 19%. Although there is no simple way to know how these finite-size effects translate to the crossover temperatures, it seems reasonable to assume that the differences between our results and [67] are caused by these finite-size effects.

In summary we believe that our results are in good agreement with the literature.

6.3.2 Comparison with Dugave, G6hmann and Kozlowski

In [70, 71] the large-distance asymptotic behaviour of the two-point functions of the XXZ chain is derived for low temperatures by summing up the asymptotically dominant terms of their expansion into form factors of the quantum transfer matrix.

By comparing this with our exact results we can establish a benchmark for the asymptotics. This will show at which distances the asymptotic expansion yields good results.

Before comparing we shall give a quick overview over the asymptotic results. First define the well known bare energy e and kernel K :

$$e(\lambda) = \text{cth}(\lambda) - \text{cth}(\lambda + \eta), \quad K(\lambda) = \text{cth}(\lambda - \eta) - \text{cth}(\lambda + \eta). \quad (6.15)$$

Then define the dressed charge Z , the density of Bethe roots ρ and the dressed energy ε :

$$Z(\lambda) = 1 + \int_{-Q}^Q \frac{d\mu}{2\pi i} K(\lambda - \mu) Z(\mu) , \quad (6.16)$$

$$\rho(\lambda) = -\frac{e(\lambda + i\gamma/2)}{2\pi i} + \int_{-Q}^Q \frac{d\mu}{2\pi i} K(\lambda - \mu) \rho(\mu) , \quad (6.17)$$

$$\varepsilon(\lambda) = \varepsilon_0(\lambda) + \int_{-Q}^Q \frac{d\mu}{2\pi i} K(\lambda - \mu) \varepsilon(\mu) , \quad \varepsilon_0(\lambda) = h - \frac{4J(1 - \Delta^2)}{\text{ch}(2\lambda) - \Delta} . \quad (6.18)$$

The two points $\pm Q$ are called the Fermi points and $Q > 0$ is determined by

$$\varepsilon(Q) = 0 . \quad (6.19)$$

In [72] it was proven that such a Q exists and is unique. With these quantities we then define the Fermi momentum k_F , the Fermi sound velocity v_0 and the dressed charge \mathcal{Z} at the Fermi point:

$$k_F = 2\pi \int_0^Q d\lambda \rho(\lambda) , \quad v_0 = \frac{\varepsilon'(Q)}{2\pi\rho(Q)} , \quad \mathcal{Z} = Z(Q) . \quad (6.20)$$

The asymptotic expressions mainly consist of products of an oscillating part and an amplitude. The amplitudes $A_{0,n}^{zz}$ and $A_{0,0}^{-+}$ are complicated expressions given in equations (90) and (97b) of [71]. The oscillating parts can easily be understood with the above definitions. For the longitudinal case the asymptotic behaviour is then described by

$$\langle \sigma_1^z \sigma_{m+1}^z \rangle - \langle \sigma_1^z \rangle \langle \sigma_{m+1}^z \rangle \sim A_{0,0}^{zz} \left(\frac{\pi T/v_0}{\text{sh}(m\pi T/v_0)} \right)^2 + A_{0,1}^{zz} \cos(2mk_F) \left(\frac{\pi T/v_0}{\text{sh}(m\pi T/v_0)} \right)^{2\mathcal{Z}^2} . \quad (6.21)$$

Here, the amplitude $A_{0,0}^{zz}$ is the leading term for $\Delta < 0$ whereas $A_{0,1}^{zz}$ is leading for $\Delta > 0$. The asymptotic behaviour for the transversal case is described by

$$\langle \sigma_1^- \sigma_{m+1}^+ \rangle \sim A_{0,0}^{-+} (-1)^m \left(\frac{\pi T/v_0}{\text{sh}(m\pi T/v_0)} \right)^{\frac{1}{2\mathcal{Z}^2}} . \quad (6.22)$$

It should be noted that these expressions are numerically efficient and can be computed on a laptop in short time. The datasets for the asymptotic parts of the plots in this section were kindly provided by Frank Göhmann and have been computed in ~ 10 minutes each.

Figure 6.14 shows the comparison between the asymptotic and exact results as functions of the distance m . It can be seen that the asymptotics come very close to the exact results for surprisingly small distances, starting

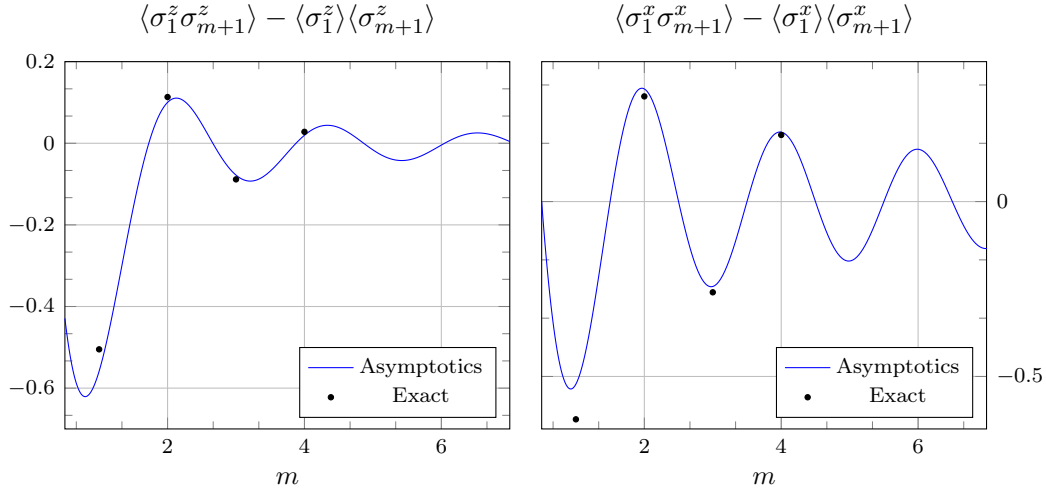


Figure 6.14: Comparison between asymptotic expansion and exact results for $\Delta = 0.6$, $h = 1$ and $T/J = 0.04$.

with $m = 3, 4$. This is of course dependent on the chosen parameters. For example, close to the isotropic point the agreement becomes worse.

Figure 6.15 shows both results as a function of the external field h . Again, for distance $m = 4$ the agreement is remarkable even for a non-trivial structure as shown for the longitudinal case. An additional comparison was done for slightly higher temperature $T/J = 0.1$, which is shown in figure 6.16. Here we can see that the phase transition at the saturation field begins to be smoothed out in the exact curve. The asymptotics do not reproduce this behaviour but still match the exact curve well apart from this point.

Figure 6.17 shows the comparison for a higher temperature ($T/J = 0.4$). Here we can see that exact and asymptotic data do not match as well as for low temperature, which is the expected behaviour since the asymptotics are derived for low temperatures. Like before, the most notable difference is near the saturation field. Apart from that the curves coincide surprisingly well.

We can conclude that the asymptotic formulae derived in [70, 71] are very close to the exact results for surprisingly small values of the distance m . A rough estimation for the temperatures for which the asymptotics are valid would be $T/J < 0.1$. In addition this comparison provides just another test to see that our results agree with other works.

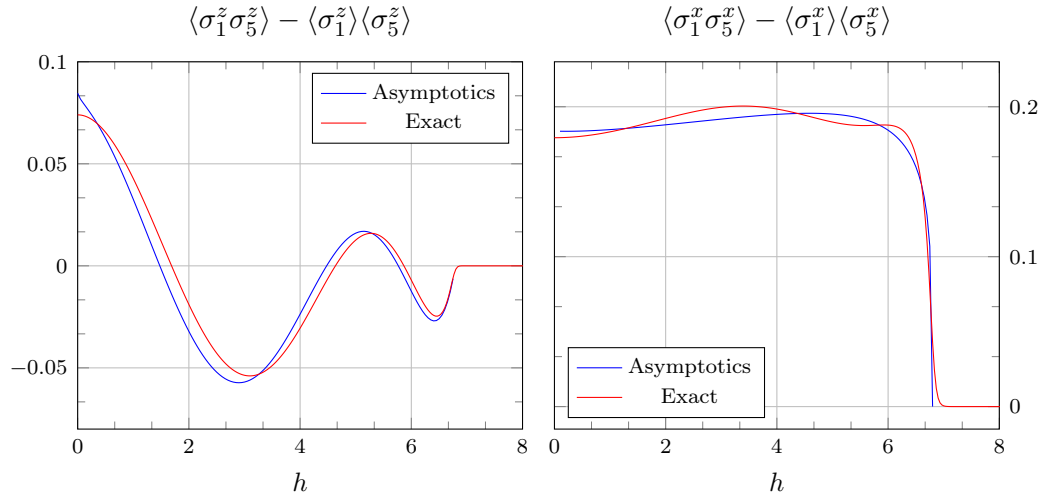


Figure 6.15: Comparison between asymptotic expansion and exact results for $\Delta = 0.7$, $T/J = 0.04$.

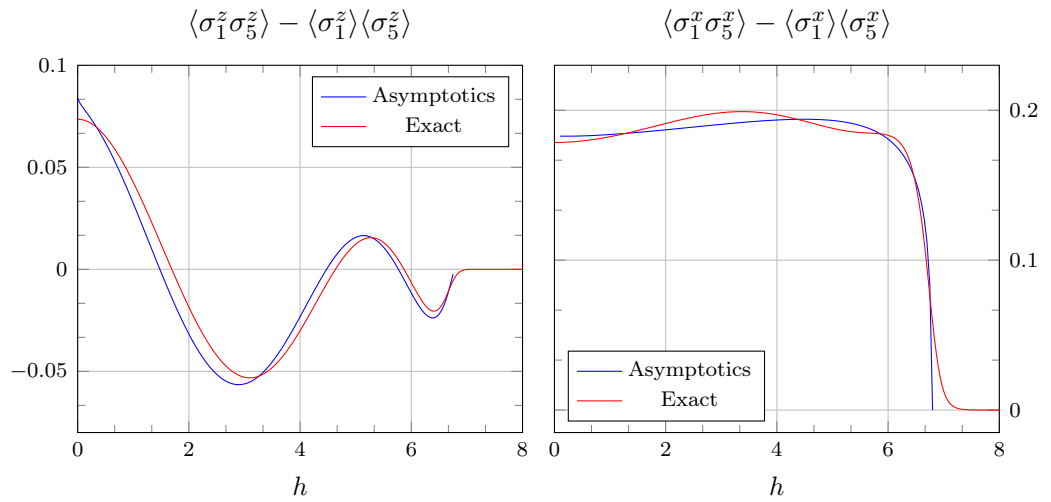


Figure 6.16: Comparison for $\Delta = 0.7$ and $T/J = 0.1$.

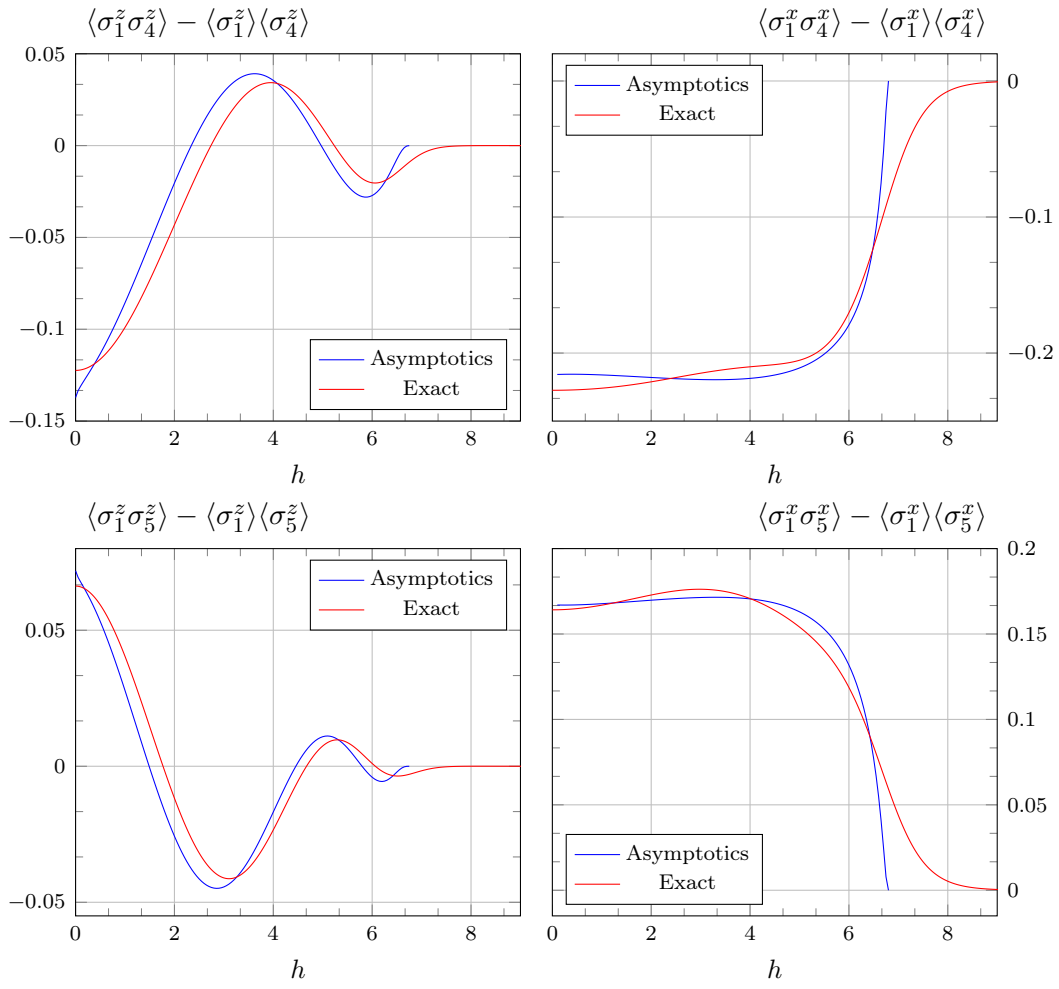


Figure 6.17: Comparison for $\Delta = 0.7$ and $T/J = 0.4$.

Chapter 7

Proof of the Exponential Form

In the following chapter we want to provide a proof that the exponential form of the density matrix explained above is correct. We will do this by using the JMS theorem which is rigorously proven in [52]. A major part of this proof is showing that a certain map

$$v^\alpha(\cdot) = \text{tr}^\alpha(e^{\Omega_0}(\cdot)) \quad (7.1)$$

acts as a dual vacuum, meaning that

$$v^\alpha(\mathbf{t}^*(\zeta)X) = 2v^\alpha(X), \quad v^\alpha(\mathbf{b}^*(\zeta)X) = v^\alpha(\mathbf{c}^*(\zeta)X) = 0. \quad (7.2)$$

This is in fact already proven in [50]. However, we feel that some points of this proof are insufficiently explained and also want to provide a more “streamlined” proof using the results of [52]. Note that there is a typo in [50] where the factor 2 is missing. Let us first give the following three definitions:

Definition.

- Generalized trace or κ -trace: For an operator $X_{[k,l]} \in M_{[k,l]}$ we define

$$\text{tr}_{[k,l]}^\kappa(X_{[k,l]}) = \frac{\text{tr}_{[k,l]}(q^{-\kappa S_{[k,l]}} X_{[k,l]})}{\text{tr}_{[k,l]}(q^{-\kappa S_{[k,l]}})}. \quad (7.3)$$

- The operator Ω_0 is the previously defined Ω were ω is replaced with ω_0 :

$$\Omega_0 = - \oint \frac{d\zeta_1^2}{2\pi i \zeta_1^2} \oint \frac{d\zeta_2^2}{2\pi i \zeta_2^2} \omega_0(\zeta_1, \zeta_2; \alpha) \mathbf{b}(\zeta_1) \mathbf{c}(\zeta_2). \quad (7.4)$$

- Function ω_0 :

$$\omega_0(\zeta, \alpha) = - \left(\frac{1 - q^\alpha}{1 + q^\alpha} \right)^2 \Delta_\zeta \psi(\zeta, \alpha). \quad (7.5)$$

We may also write $\omega_0(\zeta, \xi; \alpha) = \omega_0(\zeta/\xi, \alpha)$.

7.1 Proof of the Vacuum Property

In the following we may sometimes switch between the additive and the multiplicative representations of the spectral parameter. As before we use $\zeta = e^\lambda$ and $q = e^\eta$. Let us first proof

Lemma 1. *For a staggered choice of the inhomogeneities, i.e.*

$$\beta_j = \begin{cases} \beta_{2j-1} = \eta - \beta/N \\ \beta_{2j} = \beta/N \end{cases}$$

the functional Z^κ from [52] becomes

$$Z^\kappa \left\{ q^{2\alpha S(k-1)} X_{[k,l]} \right\} = \rho(0)^{k-1} \text{tr}_{[k,l]} \left(D_N(\kappa, \alpha) X_{[k,l]} \right) \quad (7.6)$$

where $D_N(\kappa, \alpha)$ is a homogeneous version of the generalized reduced density matrix given in [58] and N is the Trotter number.

Proof. The functional is defined by (2.5) of [52]:

$$Z^\kappa \left\{ q^{2\alpha S(k-1)} X_{[k,l]} \right\} = \rho(0)^{k-1} \frac{\langle \kappa + \alpha | \text{tr}_{[k,l]} \left(T_{[k,l],M} q^{2\kappa S_{[k,l]}} X_{[k,l]} \right) | \kappa \rangle}{\Lambda(0, \kappa)^{l-k+1} \langle \kappa + \alpha | \kappa \rangle}$$

where $\Lambda(\lambda, \kappa)$ is the eigenvalue of largest modulus of the twisted vertical transfer matrix $t(\zeta, \kappa) = \text{tr}_j \left(T_{j,M}(\zeta) q^{\kappa \sigma_j^z} \right)$. The vertical monodromy matrix is defined as

$$T_{j,M}(\lambda) = L_{j,\bar{N}}(\lambda - \beta_N) \cdots L_{j,\bar{1}}(\lambda - \beta_1)$$

where we denote the horizontal or auxiliary spaces with barred numbers. For products of monodromy matrices the shorthand notation

$$T_{[k,l],M} = T_{k,M} \cdots T_{l,M}, \quad T_{j,M} = T_{j,M}(0)$$

is used. Using staggered inhomogeneities and assuming that the Trotter number is even we obtain

$$T_{j,M} = L_{j,\bar{N}}(-\beta/N) L_{j,\overline{N-1}}(\beta/N - \eta) \cdots L_{j,\bar{2}}(-\beta/N) L_{j,\bar{1}}(\beta/N - \eta).$$

Using the crossing symmetry

$$\sigma_j^y L_{a,j}(\lambda - \eta) \sigma_j^y = b(\lambda - \eta) L_{j,a}^{t_1}(-\lambda)$$

and the definition

$$Y = \prod_{j=1}^{N/2} \sigma_{2j-1}^y$$

we obtain

$$\begin{aligned}
T_{j,M} &= L_{j,\bar{N}}(-\beta/N) b(\beta/N - \eta) \sigma_{N-1}^y L_{N-1,j}^{t_1} (-\beta/N) \sigma_{N-1}^y \cdots \\
&\quad \times L_{j,\bar{2}}(-\beta/N) b(\beta/N - \eta) \sigma_1^y L_{1,j}^{t_1} (-\beta/N) \sigma_1^y \\
&= b(\beta/N - \eta)^{N/2} Y \underbrace{L_{j,\bar{N}}(-\beta/N) L_{N-1,j}^{t_1} (-\beta/N) \cdots L_{j,\bar{2}}(-\beta/N) L_{1,j}^{t_1} (-\beta/N)}_{=T_j^{QTM}(0)=:T_j^{QTM}} Y \\
&= b(\beta/N - \eta)^{N/2} Y T_j^{QTM} Y . \\
&\Rightarrow T_{[k,l],M} = B Y T_k^{QTM} \cdots T_l^{QTM} Y
\end{aligned}$$

where $B \in \mathbb{C}$ is some prefactor containing the b 's. Inserting this into the definition of the functional we obtain

$$Z^\kappa \left\{ q^{2\alpha S(k-1)} X_{[k,l]} \right\} = \rho(0)^{k-1} \frac{\langle \kappa + \alpha | \text{tr}_{[k,l]} \left(T_{[k,l]}^{QTM} q^{2\kappa S_{[k,l]}} X_{[k,l]} \right) | \kappa \rangle}{\Lambda^{QTM}(0, \kappa)^{l-k+1} \langle \kappa + \alpha | \kappa \rangle}$$

where we used that

$$\Lambda(0, \kappa) = b(\beta/N - \eta)^{N/2} \Lambda^{QTM}(0, \kappa) .$$

Note that the vectors $\langle \kappa + \alpha |$ and $|\kappa\rangle$ are not the same as before. They now refer to the eigenvectors of the quantum transfer matrix and not the simple vertical transfer matrix as before. Comparing to equation (16) of [58] we finally arrive at

$$Z^\kappa \left\{ q^{2\alpha S(k-1)} X_{[k,l]} \right\} = \rho(0)^{k-1} \text{tr}_{[k,l]} \left(D_N(\kappa, \alpha) X_{[k,l]} \right) ,$$

where D_N is now a homogeneous version of the generalized reduced density matrix from [58] acting on the interval $[k, l]$. \square

Remark 1. Note that the prefactor $\rho(0)^{k-1}$ is consistent with the reduction relations for the density matrix given by equation (19) of [58].

Next we shall consider the limit $T \rightarrow \infty$ of the case presented above. In order to preserve as much generality as possible we will consider the case of fixed $\kappa = \frac{h}{2\eta T}$. This means of course that we will send $h \rightarrow \infty$ as well. The results for finite h may later be recovered by setting $\kappa = 0$.

Lemma 2. *In the limit $N \rightarrow \infty$ and $T \rightarrow \infty$ and for fixed κ , the functional yields the κ -trace:*

$$\lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} Z^\kappa \left\{ q^{2\alpha S(k-1)} X_{[k,l]} \right\} = \rho(0)^{k-1} \text{tr}_{[k,l]}^{-2\kappa} \left(X_{[k,l]} \right) . \quad (7.7)$$

Proof. We know that in the Trotter limit and for finite α

$$\lim_{N \rightarrow \infty} \operatorname{tr}_{[k,l]} (D_N(\kappa, \alpha) X_{[k,l]}) = \lim_{l \rightarrow \infty} \frac{\operatorname{tr}_{[-l+1,l]} (e^{-\beta H_l + 2\eta\kappa S_{[-l+1,l]}} q^{2\alpha S_{[-l+1,k-1]}} X_{[k,l]})}{\operatorname{tr}_{[-l+1,l]} (e^{-\beta H_l + 2\eta\kappa S_{[-l+1,l]}} q^{2\alpha S_{[-l+1,k-1]}})}.$$

Therefore

$$\begin{aligned} \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} Z^\kappa \left\{ q^{2\alpha S(k-1)} X_{[k,l]} \right\} &= \rho(0)^{k-1} \lim_{l \rightarrow \infty} \frac{\operatorname{tr}_{[-l+1,l]} (q^{2\kappa S_{[-l+1,l]}} q^{2\alpha S_{[-l+1,k-1]}} X_{[k,l]})}{\operatorname{tr}_{[-l+1,l]} (q^{2\kappa S_{[-l+1,l]}} q^{2\alpha S_{[-l+1,k-1]}})} \\ &= \rho(0)^{k-1} \frac{\operatorname{tr}_{[k,l]} (q^{2\kappa S_{[k,l]}} X_{[k,l]})}{\operatorname{tr}_{[k,l]} (q^{2\kappa S_{[k,l]}})} \\ &= \rho(0)^{k-1} \operatorname{tr}_{[k,l]}^{-2\kappa} (X_{[k,l]}) . \end{aligned}$$

□

Before we continue we shall consider the functions ρ and ω in the limit $T \rightarrow \infty$, as this will prove useful later. We will use the definitions of these functions from [58] which are consistent with [52] in the above case.

Lemma 3. *In the limit $T \rightarrow \infty$ and for fixed κ , the functions ρ and ω simplify to*

$$\lim_{T \rightarrow \infty} \rho(\zeta) = \frac{q^{\kappa+\alpha} + q^{-\kappa-\alpha}}{q^\kappa + q^{-\kappa}} \quad (7.8)$$

and

$$\lim_{T \rightarrow \infty} \omega(\zeta, \xi) = \left(\frac{q^\kappa - q^{-\kappa}}{q^\kappa + q^{-\kappa}} \frac{1 + q^\alpha}{1 - q^\alpha} \right)^2 \omega_0(\zeta, \xi). \quad (7.9)$$

Proof. Let us first consider the auxiliary function $\mathbf{a}(\lambda, \kappa)$ which we will need for both ρ and ω . It is defined in [58] by the non-linear integral equation

$$\ln(\mathbf{a}(\lambda, \kappa)) = -2\eta\kappa - \frac{2J\operatorname{sh}(\eta)e(\lambda)}{T} - \int_{\mathcal{C}} \frac{d\mu}{2\pi i} K(\lambda - \mu) \ln(1 + \mathbf{a}(\lambda, \kappa))$$

where

$$K(\lambda) = \operatorname{cth}(\lambda - \eta) - \operatorname{cth}(\lambda + \eta), \quad e(\lambda) = \operatorname{cth}(\lambda) - \operatorname{cth}(\lambda + \eta).$$

The integration contour is shown in figure 7.1. Then, in the limit $T \rightarrow \infty$ the driving term simplifies to only $-2\eta\kappa$. The integrand is then meromorphic and, assuming λ lies inside of \mathcal{C} , has no poles inside \mathcal{C} . Hence

$$\ln(\mathbf{a}(\lambda, \kappa)) = -2\eta\kappa \quad \Rightarrow \quad \mathbf{a}(\lambda, \kappa) = q^{-2\kappa}.$$

Now consider the function ρ . It is given by

$$\rho(\zeta) = q^\alpha \exp \left\{ \int_{\mathcal{C}} \frac{d\mu}{2\pi i} e(\mu - \lambda) \ln \left[\frac{1 + \mathbf{a}(\mu, \kappa + \alpha)}{1 + \mathbf{a}(\mu, \kappa)} \right] \right\}. \quad (7.10)$$

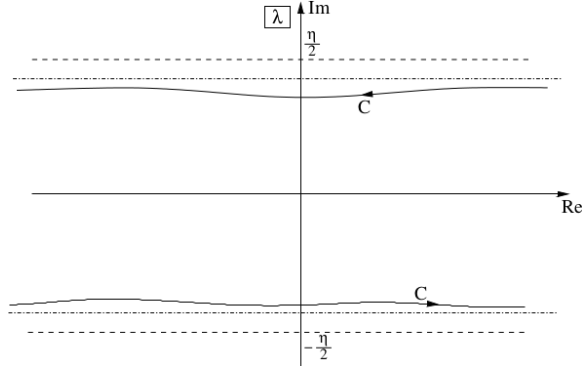


Figure 7.1: The contour \mathcal{C} surrounds the real axis in counterclockwise direction. Image from [58].

Inserting $\mathfrak{a}(\lambda, \kappa)$ and using that $e(\mu - \lambda)$ has only one pole inside \mathcal{C} which has residue 1, this simplifies to

$$\begin{aligned} \rho(\zeta) &= q^\alpha \exp \left\{ \ln \left[\frac{1 + q^{-2\kappa - 2\alpha}}{1 + q^{-2\kappa}} \right] \int_{\mathcal{C}} \frac{d\mu}{2\pi i} e(\mu - \lambda) \right\} \\ &= \frac{q^{\kappa + \alpha} + q^{-\kappa - \alpha}}{q^\kappa + q^{-\kappa}} \end{aligned}$$

which proves the first part of the lemma.

The function ω is much more complicated. We shall first give its complete representation in terms of integral equations.

$$\omega(\zeta, \xi; \kappa, \alpha) = 2\chi^\alpha \Psi(\zeta, \xi) - \Delta_\chi \psi(\chi) + 2(\rho(\zeta) - \rho(\xi))\psi(\chi)$$

where $\chi = \zeta/\xi$, ψ as before and

$$\Psi(\zeta, \xi) = \int_{\mathcal{C}} dm(\omega) G(\omega, \mu) \{ q^\alpha \text{cth}(\omega - \lambda - \eta) - \rho(\zeta) \text{cth}(\omega - \lambda) \} .$$

As usual we use $\zeta = e^\lambda$ and $\xi = e^\mu$. The integration measure is

$$dm(\lambda) = \frac{d\lambda}{2\pi i \rho(\zeta) (1 + \mathfrak{a}(\lambda, \kappa))}$$

which simplifies to

$$dm(\lambda) = \frac{d\lambda}{2\pi i \rho(\zeta) (1 + q^{-2\kappa})} .$$

The function $G(\lambda, \mu)$ is given by

$$G(\lambda, \mu) = q^{-\alpha} \text{cth}(\lambda - \mu\eta) - \rho(\xi) \text{cth}(\lambda - \mu) + \int_{\mathcal{C}} dm(\omega) K_\alpha(\lambda - \omega) G(\omega, \mu)$$

with the deformed kernel

$$K_\alpha(\lambda) = q^{-\alpha} \operatorname{cth}(\lambda - \mu) - q^\alpha \operatorname{cth}(\lambda + \mu).$$

Noting that the integrand has only one pole inside \mathcal{C} , we can conclude

$$G(\lambda, \mu) = q^{-\alpha} \operatorname{cth}(\lambda - \mu - \eta) - \rho(\xi) \operatorname{cth}(\lambda - \mu) - \frac{K_\alpha(\lambda - \mu)}{1 + q^{-2\kappa}}.$$

We can then calculate Ψ in the limit $T \rightarrow \infty$:

$$\begin{aligned} \Psi(\zeta, \xi) &= -\frac{1}{1 + q^{-2\kappa}} \{q^\alpha \operatorname{cth}(\mu - \lambda - \eta) - \rho(\zeta) \operatorname{cth}(\mu - \lambda) + G(\lambda, \mu)\} \\ &= -\frac{1}{1 + q^{-2\kappa}} \left\{ q^\alpha \operatorname{cth}(\mu - \lambda - \eta) - \rho(\zeta) \operatorname{cth}(\mu - \lambda) \right. \\ &\quad \left. + q^{-\alpha} \operatorname{cth}(\lambda - \mu - \eta) - \rho(\xi) \operatorname{cth}(\lambda - \mu) - \frac{K_\alpha(\lambda - \mu)}{1 + q^{-2\kappa}} \right\} \\ &= -\frac{1}{1 + q^{-2\kappa}} \left\{ K_\alpha(\lambda - \mu) - \frac{K_\alpha(\lambda - \mu)}{1 + q^{-2\kappa}} \right\} \\ &= -\frac{K_\alpha(\lambda - \mu)}{(q^\kappa + q^{-\kappa})^2}. \end{aligned}$$

At last we calculate ω . With $\rho(\zeta) - \rho(\xi) = 0$ in the limit $T \rightarrow \infty$ and

$$\begin{aligned} \Delta_\chi \psi(\chi) &= \frac{\chi^\alpha}{2} \left\{ q^\alpha \frac{q^2 \chi^2 + 1}{q^2 \chi^2 - 1} - q^{-\alpha} \frac{q^{-2} \chi^2 + 1}{q^{-2} \chi^2 - 1} \right\} \\ &= \frac{\chi^\alpha}{2} \{q^\alpha \operatorname{cth}(\lambda - \mu + \eta) - q^{-\alpha} \operatorname{cth}(\lambda - \mu - \eta)\} \\ &= -\frac{\chi^\alpha}{2} K_\alpha(\lambda - \mu) \end{aligned}$$

we conclude

$$\begin{aligned} \omega(\zeta, \xi; \kappa, \alpha) &= \frac{\chi^\alpha}{2} \left\{ 1 - \frac{4}{(q^\kappa + q^{-\kappa})^2} K_\alpha(\lambda - \mu) \right\} \\ &= \frac{\chi^\alpha}{2} \left(\frac{q^\kappa - q^{-\kappa}}{q^\kappa + q^{-\kappa}} \right)^2 K_\alpha(\lambda - \mu). \end{aligned}$$

Now only the comparison to ω_0 remains:

$$\begin{aligned} \omega_0(\zeta, \alpha) &= -\left(\frac{1 - q^\alpha}{1 + q^\alpha} \right)^2 \underbrace{\Delta_\zeta \psi(\zeta, \alpha)}_{= -\frac{\zeta^\alpha}{2} K_\alpha(\lambda)} \\ &= \frac{\zeta^\alpha}{2} \left(\frac{1 - q^\alpha}{1 + q^\alpha} \right)^2 K_\alpha(\lambda), \end{aligned}$$

which proves part two of the lemma. \square

We are now able to prove a homogeneous version of lemma 5.2 of [50]. Note that this lemma makes statements about operators acting on a finite chain while [52] considers the infinite chain.

Lemma 4. *For any local operator $X_{[k,l]} \in M_{[k,l]}$ we have*

$$\mathrm{tr}_{[k,l+m]}^{-2\kappa} \left(\mathbf{t}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right) = 2 \frac{q^{\kappa+\alpha} + q^{-\kappa-\alpha}}{q^\kappa + q^{-\kappa}} \mathrm{tr}_{[k,l]}^{-2\kappa} (X_{[k,l]}) \quad \text{mod } (\zeta^2 - 1)^m \quad (7.11)$$

and

$$\begin{aligned} \mathrm{tr}_{[k,l+m]}^{-2\kappa} \left(\mathbf{b}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right) &= \left(\frac{q^\kappa - q^{-\kappa}}{q^\kappa + q^{-\kappa}} \frac{1 + q^\alpha}{1 - q^\alpha} \right)^2 \\ &\times \oint_{\Gamma} \frac{d\xi^2}{2\pi i \xi^2} \omega_0(\zeta, \xi; \alpha) \mathrm{tr}_{[k,l]}^{-2\kappa} (\mathbf{c}_{[k,l]}(\xi, \alpha) X_{[k,l]}) \quad \text{mod } (\zeta^2 - 1)^m . \end{aligned}$$

Proof. To prove the first equation we shall use

$$Z^\kappa \{ \mathbf{t}^*(\zeta) X \} = 2\rho(\zeta) Z^\kappa \{ X \}$$

which is shown in [52] for a quasi-local $X \in \mathcal{W}^{(\alpha)}$. In the following we shall consider the staggered choice of inhomogeneities explained above and also take the limits $N \rightarrow \infty$ and $T \rightarrow \infty$. As explained earlier in section 3.1, setting $X^{(s)} = q^{2(\alpha-s)S(k-1)} X_{[k,l]}^{(s)} \in \mathcal{W}_{\alpha-s,s}$ where $X_{[k,l]}^{(s)} \in M_{[k,l]}$ and $\mathbb{S}(X_{[k,l]}^{(s)}) = s$, equation (3.12) is true. Inserting this into the above equation we obtain

$$\begin{aligned} \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} l.h.s &= \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} Z^\kappa \left\{ \mathbf{t}^*(\zeta) q^{2\alpha S(k-1)} X_{[k,l]} \right\} \\ &= \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} Z^\kappa \left\{ q^{2\alpha S(k-1)} \mathbf{t}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right\} \quad \text{mod } (\zeta^2 - 1)^m \\ &= \rho(0)^{k-1} \mathrm{tr}_{[k,l+m]}^{-2\kappa} \left(\mathbf{t}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right) \quad \text{mod } (\zeta^2 - 1)^m . \end{aligned}$$

We have restricted ourselves to the case $\mathbb{S}(X) = 0$, because any operator with non-zero spin will vanish under the trace. The right-hand side directly becomes

$$\lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} r.h.s = 2 \frac{q^{\kappa+\alpha} + q^{-\kappa-\alpha}}{q^\kappa + q^{-\kappa}} \rho(0)^{k-1} \mathrm{tr}_{[k,l]}^{-2\kappa} (X_{[k,l]})$$

in the limit $T \rightarrow \infty$, which proves the first equation.

For the second equation we then shall use

$$Z^\kappa \{ \mathbf{b}^*(\zeta) X \} = \oint_{\Gamma} \frac{d\xi^2}{2\pi i \xi^2} \omega(\zeta, \xi) Z^\kappa \{ \mathbf{c}(\xi) X \} .$$

Similar to above we shall only consider operators of spin $\mathbb{S}(X) = -1$ for the same reason. It follows

$$\begin{aligned} \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} l.h.s. &= \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} Z^\kappa \left\{ \mathbf{b}^*(\zeta) q^{2(\alpha+1)S(k-1)} X_{[k,l]} \right\} \\ &= \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} Z^\kappa \left\{ q^{2\alpha S(k-1)} \mathbf{b}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right\} \pmod{(\zeta^2 - 1)^m} \\ &= \rho(0)^{k-1} \text{tr}_{[k,l+m]}^{-2\kappa} \left(\mathbf{b}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right) \pmod{(\zeta^2 - 1)^m}. \end{aligned}$$

On the right-hand side we need to consider annihilation operators for which we will use equation (3.7). Then, similar to above we obtain

$$\begin{aligned} \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} r.h.s. &= \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} \oint_{\Gamma} \frac{d\xi^2}{2\pi i \xi^2} \omega(\zeta, \xi) Z^\kappa \left\{ \mathbf{c}(\xi) q^{2(\alpha+1)S(k-1)} X_{[k,l]} \right\} \\ &= \lim_{\substack{N \rightarrow \infty \\ T \rightarrow \infty}} \oint_{\Gamma} \frac{d\xi^2}{2\pi i \xi^2} \omega(\zeta, \xi) Z^\kappa \left\{ q^{2\alpha S(k-1)} \mathbf{c}_{[k,l]}(\xi, \alpha) X_{[k,l]} \right\} \\ &= \oint_{\Gamma} \frac{d\xi^2}{2\pi i \xi^2} \left(\frac{q^\kappa - q^{-\kappa} 1 + q^\alpha}{q^\kappa + q^{-\kappa} 1 - q^\alpha} \right)^2 \omega_0(\zeta, \xi; \alpha) \rho(0)^{k-1} \text{tr}_{[k,l]}^{-2\kappa} \left(\mathbf{c}_{[k,l]}(\xi, \alpha) X_{[k,l]} \right). \end{aligned}$$

□

Remark 1. Of course there is a similar relation for the operators \mathbf{c}^* and \mathbf{b} which reads

$$\begin{aligned} \text{tr}_{[k,l+m]}^{-2\kappa} \left(\mathbf{c}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right) &= - \left(\frac{q^\kappa - q^{-\kappa} 1 + q^\alpha}{q^\kappa + q^{-\kappa} 1 - q^\alpha} \right)^2 \\ &\times \oint_{\Gamma} \frac{d\xi^2}{2\pi i \xi^2} \omega_0(\xi, \zeta; \alpha) \text{tr}_{[k,l]}^{-2\kappa} \left(\mathbf{b}_{[k,l]}(\xi, \alpha) X_{[k,l]} \right) \pmod{(\zeta^2 - 1)^m}. \end{aligned} \quad (7.12)$$

It can be obtained using the according relation from [52] or by applying the map ϕ to lemma 4.

Remark 2. In the above proof we used a crucial convention of [52]. As we know the creation operators have the block structure

$$\begin{aligned} \mathbf{t}^* &: \mathcal{W}_{\alpha-s,s} \rightarrow \mathcal{W}_{\alpha-s,s}, \\ \mathbf{b}^* &: \mathcal{W}_{\alpha-s+1,s-1} \rightarrow \mathcal{W}_{\alpha-s,s}, \quad \mathbf{c}^* : \mathcal{W}_{\alpha-s-1,s+1} \rightarrow \mathcal{W}_{\alpha-s,s}. \end{aligned}$$

This implies that the functions ρ and ω in the JMS theorem depend on the values $\alpha - s$ or rather α since we consider the $s = 0$ sector. In other words, the functions generally do not depend on the same parameter as an operator X but rather share the parameter of the complete operator on which the functional acts. This fact becomes clear by applying the JMS theorem on the definition of the function ω :

$$\omega(\zeta, \xi; \alpha) = Z^\kappa \left\{ \mathbf{b}^*(\zeta) \mathbf{c}^*(\xi) q^{2\alpha S(0)} \right\}.$$

Next we want to expand lemma 4 to the infinite case. In order to do this, let us first consider how to expand the κ -trace. Suppose $-l+1 \leq k \leq m \leq l$. Then

$$\begin{aligned}
\mathrm{tr}_{[k,m]}^{-2\kappa} (X_{[k,m]}) &= \frac{\mathrm{tr}_{[k,m]} (q^{2\kappa S_{[k,m]}} X_{[k,m]})}{\mathrm{tr}_{[k,m]} (q^{2\kappa S_{[k,m]}})} \\
&= \frac{\mathrm{tr}_{[-l+1,l]} (q^{2\kappa S_{[-l+1,l]}} q^{2\alpha S_{[-l+1,k-1]}} X_{[k,m]})}{\mathrm{tr}_{[-l+1,l]} (q^{2\kappa S_{[-l+1,l]}} q^{2\alpha S_{[-l+1,k-1]}})} \\
&= \frac{\mathrm{tr}_{[-l+1,l]} (q^{2\kappa S_{[-l+1,l]}})}{\mathrm{tr}_{[-l+1,l]} (q^{2\kappa S_{[-l+1,l]}} q^{2\alpha S_{[-l+1,k-1]}})} \mathrm{tr}_{[-l+1,l]}^{-2\kappa} (q^{2\alpha S_{[-l+1,k-1]}} X_{[k,m]}) \\
&= \left(\frac{q^\kappa + q^{-\kappa}}{q^{\kappa+\alpha} + q^{-\kappa-\alpha}} \right)^{k+l-1} \mathrm{tr}_{[-l+1,l]}^{-2\kappa} (q^{2\alpha S_{[-l+1,k-1]}} X_{[k,m]}) \\
&= \rho^{-k-l+1} \mathrm{tr}_{[-l+1,l]}^{-2\kappa} (q^{2\alpha S_{[-l+1,k-1]}} X_{[k,m]}) . \tag{7.13}
\end{aligned}$$

We would now like to define the κ -trace on the infinite chain sending $l \rightarrow \infty$. This is obviously not generally possible. If we set $\kappa = -\alpha/2$ however, we obtain

$$\mathrm{tr}_{[k,m]}^\alpha (X_{[k,m]}) = \mathrm{tr}_{[-l+1,l]}^\alpha (q^{2\alpha S_{[-l+1,k-1]}} X_{[k,m]}) \tag{7.14}$$

and can then define the κ -trace on a quasi-local operator $q^{2\alpha S^{(k-1)}} X_{[k,l]} \in \mathcal{W}^{(\alpha)}$:

$$\mathrm{tr}^\alpha (q^{2\alpha S^{(k-1)}} X_{[k,l]}) = \mathrm{tr}_{[k,l]}^\alpha (X_{[k,l]}) . \tag{7.15}$$

Using this we can now prove

Lemma 5. *For a quasi-local operator X , we have*

$$\mathrm{tr}^\alpha (\mathbf{t}^*(\zeta)X) = 2 \mathrm{tr}^\alpha (X) , X \in \mathcal{W}_\alpha , \tag{7.16a}$$

$$\mathrm{tr}^\alpha (\mathbf{b}^*(\zeta)X) = \oint_\Gamma \frac{d\xi^2}{2\pi i \xi^2} \omega_0(\zeta, \xi; \alpha) \mathrm{tr}^\alpha (\mathbf{c}(\xi)X) , X \in \mathcal{W}_{\alpha+1} , \tag{7.16b}$$

$$\mathrm{tr}^\alpha (\mathbf{c}^*(\zeta)X) = - \oint_\Gamma \frac{d\xi^2}{2\pi i \xi^2} \omega_0(\xi, \zeta; \alpha) \mathrm{tr}^\alpha (\mathbf{b}(\xi)X) , X \in \mathcal{W}_{\alpha-1} . \tag{7.16c}$$

Proof. All three equations are proven by taking lemma 4, setting $\kappa = -\alpha/2$ and then expanding the trace to the infinite chain. As before, we will restrict the spin to 0 or ± 1 . Let us consider the first equation of lemma 4:

$$\begin{aligned}
l.h.s &= \mathrm{tr}_{[k,l+m]}^\alpha \left(\mathbf{t}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right) \\
&= \mathrm{tr}^\alpha \left(q^{2\alpha S^{(k-1)}} \mathbf{t}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right) \\
&= \mathrm{tr}^\alpha \left(\mathbf{t}^*(\zeta) q^{2\alpha S^{(k-1)}} X_{[k,l]} \right) \pmod{(\zeta^2 - 1)^m}
\end{aligned}$$

and

$$r.h.s = 2 \mathrm{tr}_{[k,l]}^\alpha (X_{[k,l]}) = \mathrm{tr}^\alpha (q^{2\alpha S^{(k-1)}} X_{[k,l]})$$

which proves the first equation.

The second equation is proven similarly. The factor before the integral in lemma 4(ii) reduces to one when we set $\kappa = -\alpha/2$. We obtain

$$\begin{aligned} l.h.s &= \text{tr}_{[k,l+m]}^\alpha \left(\mathbf{b}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right) \\ &= \text{tr}^\alpha \left(q^{2\alpha S(k-1)} \mathbf{b}_{[k,l+m]}^*(\zeta, \alpha) X_{[k,l]} \right) \\ &= \text{tr}^\alpha \left(\mathbf{b}^*(\zeta) q^{2(\alpha+1)S(k-1)} X_{[k,l]} \right) \pmod{(\zeta^2 - 1)^m} \end{aligned}$$

and

$$\text{tr}_{[k,l]}^\alpha \left(\mathbf{c}_{[k,l]}(\xi, \alpha) X_{[k,l]} \right) = \text{tr}^\alpha \left(\mathbf{c}(\xi) q^{2(\alpha+1)S(k-1)} X_{[k,l]} \right).$$

Inserting into lemma 4 proves the second equation.

The third part can then be proven completely analogously to the second part. \square

Note that it would of course be possible to leave out lemma 4 and just prove lemma 5 using the JMS theorem directly. We feel however that the distinctions presented can be a source of confusion and therefore preferred to present both cases.

We are now ready to prove

Theorem 1. *The map $\text{tr}^\alpha (e^{\Omega_0}(\cdot))$ acts as the dual vacuum on any quasi-local operator $X \in \mathcal{W}^{(\alpha)}$, i.e.*

$$\text{tr}^\alpha (e^{\Omega_0} \mathbf{t}^*(\zeta) X) = 2 \text{tr}^\alpha (e^{\Omega_0} X), \quad (7.17a)$$

$$\text{tr}^\alpha (e^{\Omega_0} \mathbf{b}^*(\zeta) X) = 0, \quad (7.17b)$$

$$\text{tr}^\alpha (e^{\Omega_0} \mathbf{c}^*(\zeta) X) = 0. \quad (7.17c)$$

Proof. The first equation follows easily from lemma 5 and the fact that \mathbf{t}^* commutes with the fermionic operators:

$$\text{tr}^\alpha (e^{\Omega_0} \mathbf{t}^*(\zeta) X) = \text{tr}^\alpha (\mathbf{t}^*(\zeta) e^{\Omega_0} X) = 2 \text{tr}^\alpha (e^{\Omega_0} X).$$

To prove the second and third equations we shall consider a quasi-local operator $Y \in \mathcal{W}^{(\alpha)}$ which is constructed as follows:

$$Y = \mathcal{B}^{(n)} \mathcal{C}^{(n)} q^{2\alpha S(k-1)}$$

where

$$\mathcal{B}^{(n)} = \mathbf{b}^*(\zeta_n) \cdots \mathbf{b}^*(\zeta_1), \quad \mathcal{C}^{(n)} = \mathbf{c}^*(\xi_n) \cdots \mathbf{c}^*(\xi_1).$$

Because of the first equation we may disregard any \mathbf{t}^* . If an operator Y were of the form $\mathcal{B}^{(n)} \mathcal{C}^{(m)} q^{2\alpha S(k-1)}$ where $n \neq m$, i.e. being ‘‘unbalanced’’ in the number of \mathbf{b}^* 's and \mathbf{c}^* 's, it would be mapped to zero:

$$\text{tr}^\alpha \left(e^{\Omega_0} \mathcal{B}^{(n)} \mathcal{C}^{(m)} q^{2\alpha S(k-1)} \right) = 0, \quad \text{for } n \neq m.$$

This is simply because such an operator has a non-zero spin. As such, we may always assume, without loss of generality, that any operator $Y = \mathbf{x}^*(\zeta)X \in \mathcal{W}^{(\alpha)}$ can be represented in the above way (where $n = m$). Let $\mathcal{C}_j^{(n)}$ denote $\mathcal{C}^{(n)}$ where the j -th factor is omitted. Then consider

$$\begin{aligned}
\mathrm{tr}^\alpha(\Omega_0 Y) &= \oint_\Gamma \frac{dx^2}{2\pi i x^2} \oint_\Gamma \frac{dz^2}{2\pi i z^2} \omega_0(z, x) \mathrm{tr}^\alpha \left(\mathbf{b}(z) \mathbf{c}(x) \mathcal{B}^{(n)} \mathcal{C}^{(n)} q^{2\alpha S(k-1)} \right) \\
&= - \oint_\Gamma \frac{dx^2}{2\pi i x^2} \mathrm{tr}^\alpha \left(\mathbf{c}^*(x) \mathbf{c}(x) \mathcal{B}^{(n)} \mathcal{C}^{(n)} q^{2\alpha S(k-1)} \right) \\
&= - \oint_\Gamma \frac{dx^2}{2\pi i x^2} \mathrm{tr}^\alpha \left((-1)^n \mathbf{c}^*(x) \mathcal{B}^{(n)} \sum_{j=1}^n (-1)^{n-j} \psi(x/\xi_j) \mathcal{C}_j^{(n)} q^{2\alpha S(k-1)} \right) \\
&= - \mathrm{tr}^\alpha \left((-1)^n \sum_{j=1}^n (-1)^{n-j} \mathbf{c}^*(\xi_j) \mathcal{B}^{(n)} \mathcal{C}_j^{(n)} q^{2\alpha S(k-1)} \right) \\
&= - \sum_{j=1}^n (-1)^{n-j} \mathrm{tr}^\alpha \left(\mathcal{B}^{(n)} \underbrace{\mathbf{c}^*(\xi_j) \mathcal{C}_j^{(n)}}_{=(-1)^{n-j} \mathcal{C}^{(n)}} q^{2\alpha S(k-1)} \right) \\
&= - \sum_{j=1}^n \mathrm{tr}^\alpha \left(\mathcal{B}^{(n)} \mathcal{C}^{(n)} q^{2\alpha S(k-1)} \right) \\
&= -n \mathrm{tr}^\alpha(Y).
\end{aligned}$$

Here we used lemma 5 at the top.

Since the operator $\Omega_0^m Y$ is equal to a linear combination of operators of the form $\mathcal{B}^{(n-m)} \mathcal{C}^{(n-m)} q^{2\alpha S(k-1)}$, we obtain for $0 \leq m \leq n$ using linearity,

$$\begin{aligned}
\mathrm{tr}^\alpha(\Omega_0^m Y) &= -(n-m+1) \mathrm{tr}^\alpha(\Omega_0^{m-1} Y) \\
&= (-1)^m \frac{n!}{(n-m)!} \mathrm{tr}^\alpha(Y).
\end{aligned}$$

It then follows

$$\begin{aligned}
\mathrm{tr}^\alpha(e^{\Omega_0} Y) &= \sum_{m=0}^n \mathrm{tr}^\alpha \left(\frac{\Omega_0^m}{m!} Y \right) \\
&= \sum_{m=0}^n (-1)^m \binom{n}{m} \mathrm{tr}^\alpha(Y) \\
&= \begin{cases} 1 & , n = 0 \\ 0 & , n \neq 0. \end{cases}
\end{aligned}$$

which proves the second and third equations. \square

7.2 Expectation Values for Vanishing External Field

We can now prove that the exponential form indeed produces correct expectation values. We shall however restrict ourselves to one of two cases: first the case of a vanishing external field ($h = 0$) and second the case of operators which are even under spin reversal, i.e. $\mathbb{J}(X) = X$.

The motivation to consider these two cases comes from [53]. The reason is that in these two cases the operator Ω_2 vanishes. Even though this operator is not rigorously proven to render correct results, the authors of [53] have confirmed that $\langle X \rangle_{T,h} = \lim_{\alpha \rightarrow 0} \text{tr}^\alpha (e^{\Omega_1 + \Omega_2} X)$ by comparing with various known results. For the first case it is easy to see that Ω_2 vanishes: since the eigenvalue $\Lambda(\zeta, \kappa)$ is even in κ (see [58]) the function φ has to be uneven in κ and therefore zero for $\kappa = h = 0$.

The second case is less obvious: we know that for an operator X even under spin reversal, the expectation value is even in h : $\langle X \rangle_{T,h} = \langle X \rangle_{T,-h}$. For finite α there is a similar property:

$$\text{tr}^\alpha \left(e^{\Omega_1(\kappa, \alpha) + \Omega_2(\kappa, \alpha)} X \right) = \text{tr}^{-\alpha} \left(e^{\Omega_1(-\kappa, -\alpha) + \Omega_2(-\kappa, -\alpha)} X \right). \quad (7.18)$$

Since Ω_2 is nilpotent ($\Omega_2^2 = 0$) and thus $e^{\Omega_2} = 1 + \Omega_2$ it follows that

$$\text{tr}^\alpha (e^{\Omega_1 + \Omega_2} X) = \text{tr}^\alpha (e^{\Omega_1} X) + \text{tr}^\alpha (\Omega_2 e^{\Omega_1} X). \quad (7.19)$$

Using the properties $\omega(\zeta, \xi; \kappa, \alpha) = \omega(\zeta, \xi; -\kappa, -\alpha)$ and $\varphi(\zeta; \kappa, \alpha) = -\varphi(\zeta; -\kappa, -\alpha)$, it follows that $\lim_{\alpha \rightarrow 0} \text{tr}^\alpha (\Omega_2 e^{\Omega_1} X) = 0$ and thus

$$\langle X \rangle_{T,h} = \lim_{\alpha \rightarrow 0} \text{tr}^\alpha (e^{\Omega_1} X), \quad (7.20)$$

showing that Ω_2 is not needed in the second case as well.

We shall now prove

Theorem 2. *For a quasi-local operator $X \in \mathcal{W}^{(\alpha)}$, in the case of a vanishing external field, thermal expectation values are given by*

$$\langle X \rangle_{T,h=0} = \lim_{\alpha \rightarrow 0} \text{tr}^\alpha (e^{\Omega_1} X). \quad (7.21)$$

Proof. Let us consider an operator

$$Y = \mathbf{t}^*(\theta_1) \cdots \mathbf{t}^*(\theta_k) X, \quad X = \mathcal{B}^{(n)} \mathcal{C}^{(n)} q^{2\alpha S(k-1)}.$$

Like before, without loss of generality we restrict ourselves to the spin zero case. Also set $\tilde{\Omega} = \Omega_1 - \Omega_0$, then

$$\text{tr}^\alpha (e^{\Omega_1} Y) = \text{tr}^\alpha (e^{\Omega_0} e^{\tilde{\Omega}} Y) = v^\alpha (e^{\tilde{\Omega}} Y).$$

It is then immediately clear that

$$v^\alpha (e^{\tilde{\Omega}} Y) = 2^k v^\alpha (e^{\tilde{\Omega}} X).$$

Since the operator $\tilde{\Omega}^m X$ is equal to a linear combination of operators of the form $\mathcal{B}^{(n-m)} \mathcal{C}^{(n-m)} q^{2\alpha S(k-1)}$ and due to the dual vacuum property of v^α it follows that

$$v^\alpha \left(e^{\tilde{\Omega} Y} \right) = 2^k \sum_{m=0}^n \frac{1}{m!} v^\alpha \left(\tilde{\Omega}^m X \right) = \frac{2^k}{n!} v^\alpha \left(\tilde{\Omega}^n X \right).$$

Now set $\tilde{\omega} = \omega - \omega_0$ and $\sigma_m^n = (m, m+1, \dots, n)$ and consider

$$\begin{aligned} \mathbf{b}(z) \mathcal{B}^{(n)} q^{2\alpha S(k-1)} &= \sum_{i=1}^n (-1)^{i+1} (-\psi(\zeta_i/z)) \mathcal{B}_i^{(n)} q^{2\alpha S(k-1)}, \\ \mathbf{b}(z) \mathcal{B}_l^{(n)} q^{2\alpha S(k-1)} &= \sum_{i=1}^{n-1} (-1)^{i+1} \left(-\psi \left(\zeta_{\sigma_l^n(i)} / z \right) \right) \mathcal{B}_{l, \sigma_l^n(i)}^{(n)} q^{2\alpha S(k-1)} \end{aligned}$$

and

$$\begin{aligned} \mathbf{c}(x) \mathcal{C}^{(n)} q^{2\alpha S(k-1)} &= \sum_{i=1}^n (-1)^{n-i} \psi(x/\xi_i) \mathcal{C}_i^{(n)} q^{2\alpha S(k-1)}, \\ \mathbf{c}(x) \mathcal{C}_l^{(n)} q^{2\alpha S(k-1)} &= \sum_{i=1}^{n-1} (-1)^{n-i-1} \psi \left(x / \xi_{\sigma_l^n(i)} \right) \mathcal{C}_{l, \sigma_l^n(i)}^{(n)} q^{2\alpha S(k-1)}. \end{aligned}$$

It then follows that

$$\begin{aligned} &\tilde{\Omega} \mathcal{B}^{(n)} \mathcal{C}^{(n)} q^{2\alpha S(k-1)} \\ &= - \oint_{\Gamma} \frac{dz^2}{2\pi i z^2} \oint_{\Gamma} \frac{dx^2}{2\pi i x^2} \tilde{\omega}(z, x) \mathbf{b}(z) \mathbf{c}(x) \mathcal{B}^{(n)} \mathcal{C}^{(n)} q^{2\alpha S(k-1)} \\ &= - \oint_{\Gamma} \frac{dz^2}{2\pi i z^2} \oint_{\Gamma} \frac{dx^2}{2\pi i x^2} \tilde{\omega}(z, x) (-1)^n \\ &\quad \times \left[\sum_{i=1}^n (-1)^{i+1} (-\psi(\zeta_i/z)) \mathcal{B}_i^{(n)} \right] \left[\sum_{j=1}^n (-1)^{n-j} \psi(x/\xi_j) \mathcal{C}_j^{(n)} \right] \\ &= \sum_{i,j=1}^n (-1)^{i+j} \tilde{\omega}(\zeta_i, \xi_j) \mathcal{B}_i^{(n)} \mathcal{C}_j^{(n)} q^{2\alpha S(k-1)} \end{aligned}$$

and similarly

$$\tilde{\Omega} \mathcal{B}_l^{(n)} \mathcal{C}_m^{(n)} q^{2\alpha S(k-1)} = \sum_{i,j=1}^{n-1} (-1)^{i+j} \tilde{\omega} \left(\zeta_{\sigma_l^n(i)}, \xi_{\sigma_m^n(j)} \right) \mathcal{B}_{l, \sigma_l^n(i)}^{(n)} \mathcal{C}_{m, \sigma_m^n(j)}^{(n)}.$$

We can now prove by induction that

$$\tilde{\Omega}^n \mathcal{B}^{(n)} \mathcal{C}^{(n)} q^{2\alpha S(k-1)} = n! \det \left(\tilde{\omega}(\zeta_i, \xi_j) \right)_{i,j=1, \dots, n} q^{2\alpha S(k-1)}. \quad (7.22)$$

Clearly this is true for $n = 1$. To perform the induction step consider

$$\begin{aligned}
& \tilde{\Omega}^{n+1} \mathcal{B}^{(n+1)} \mathcal{C}^{(n+1)} q^{2\alpha S(k-1)} \\
&= \sum_{i,j=1}^{n+1} (-1)^{i+j} \tilde{\omega}(\zeta_i, \xi_j) \tilde{\Omega}^n \mathcal{B}_i^{(n)} \mathcal{C}_j^{(n)} q^{2\alpha S(k-1)} \\
&= \sum_{i,j=1}^{n+1} (-1)^{i+j} \tilde{\omega}(\zeta_i, \xi_j) n! \det \left(\tilde{\omega}(\zeta_{\sigma_i^{n+1}(l)}, \xi_{\sigma_j^{n+1}(m)}) \right)_{l,m=1,\dots,n} \\
&= n! \sum_{i=1}^{n+1} \sum_{j=1}^{n+1} (-1)^{i+j} \tilde{\omega}(\zeta_i, \xi_j) \det \left(\tilde{\omega}(\zeta_{\sigma_i^{n+1}(l)}, \xi_{\sigma_j^{n+1}(m)}) \right)_{l,m=1,\dots,n} \\
&= n! \sum_{i=1}^{n+1} \det (\tilde{\omega}(\zeta_l, \xi_m))_{l,m=1,\dots,n+1} \\
&= (n+1)! \det (\tilde{\omega}(\zeta_i, \xi_j))_{i,j=1,\dots,n+1} ,
\end{aligned}$$

which proves (7.22). Here we are able to use Laplace's expansion because σ is the permutation that connects a matrix A to its minor matrix A_{ij} .

It is then clear that

$$\mathrm{tr}^\alpha (e^{\Omega_1} Y) = 2^k \det (\tilde{\omega}(\zeta_i, \xi_j))_{i,j=1,\dots,n} . \quad (7.23)$$

We obtain the same expression if we take $Z^\kappa \{Y\}$ and use the JMS theorem. Since this theorem is valid for any κ and α we may choose $\kappa = -\alpha/2$, which sets $\rho(\zeta) = 1$, and then send $\alpha \rightarrow 0$. Since this means that $\kappa \rightarrow 0$ as well, this proves the theorem in the case of a vanishing external field. \square

7.3 Operators Even Under Spin Reversal and the Operator $\mathbf{t}(\zeta)$

Next we want to cover the case of an operator even under spin reversal. As mentioned before, the construction given in [53] is not rigorously proven. We also cannot give a complete proof for the exponential form. However, we think that it might be helpful to establish a link between our problem and the so-called missing \mathbf{t} operator.

The proposed \mathbf{t} operator would form a pair with \mathbf{t}^* like the fermionic operators \mathbf{c}, \mathbf{c}^* and \mathbf{b}, \mathbf{b}^* . Intuitively one would assume \mathbf{t}, \mathbf{t}^* to be bosons commuting with the fermionic operators. The operator \mathbf{t} proposed in [58] is however more complicated. As a starting point we shall define Ω_2 in terms of \mathbf{t} . In the above work

$$\Omega_2 = \oint \frac{d\zeta^2}{2\pi i \zeta^2} \ln(\rho(\zeta)) \mathbf{t}(\zeta) \quad (7.24)$$

is proposed. Starting from this the authors derive some properties that \mathbf{t} would need to obey so that the exponential form can give the complete density matrix. This is done for the inhomogeneous case. The existence of the \mathbf{t} operator could not be proven for the general case so far. However, as explained in [58], for $n = 1, 2, 3$ an operator \mathbf{t} can be constructed that obeys all required properties. This fact is remarkable, since the associated system of equations that \mathbf{t} needs to solve is strongly overdetermined. We would like to derive the properties that an operator \mathbf{t} would need to have in the homogeneous case and then follow that Ω_2 is not needed to calculate the expectation value of an operator which is even under spin reversal. This obviously will not give us a definite proof but instead a conjecture for our statement. The only non-proven assumption would be the existence of \mathbf{t} . But according to [58] there is evidence that \mathbf{t} does exist.

For an operator $X = \mathcal{B}^{(n)}\mathcal{C}^{(n)}q^{2\alpha S(0)} \in \mathcal{W}^{(\alpha)}$ we require Ω_2 to obey

$$\mathrm{tr}^\alpha \left(e^{\Omega_1 + \Omega_2} \mathbf{t}^*(\theta_1) \dots \mathbf{t}^*(\theta_m) X \right) = \left(\prod_{j=1}^m 2\rho(\theta_j) \right) \mathrm{tr}^\alpha \left(e^{\Omega_0} e^{\tilde{\Omega}} X \right). \quad (7.25)$$

Using the above definition of Ω_2 suppose that

$$\mathbf{t}(\zeta) \mathbf{t}^*(\theta) - \mathbf{t}^*(\theta) \mathbf{t}(\zeta) = -(\zeta/\theta)^\alpha \psi(\theta/\zeta, \alpha) \mathbf{t}^*(\theta). \quad (7.26)$$

Setting $\mathcal{T}_{k\dots l}^* = \mathbf{t}^*(\theta_k) \dots \mathbf{t}^*(\theta_l)$ it would then follow that

$$\begin{aligned} & \Omega_2 \mathcal{T}_{1\dots m}^* \\ &= \oint \frac{d\zeta^2}{2\pi i \zeta^2} \ln(\rho(\zeta)) \mathbf{t}(\zeta) \mathcal{T}_{1\dots m}^* \\ &= \oint \frac{d\zeta^2}{2\pi i \zeta^2} \frac{1}{2} \frac{\zeta^2 + \theta_1^2}{\zeta^2 - \theta_1^2} \ln(\rho(\zeta)) \mathcal{T}_{1\dots m}^* + \oint \frac{d\zeta^2}{2\pi i \zeta^2} \ln(\rho(\zeta)) \mathbf{t}^*(\theta_1) \mathbf{t}(\zeta) \mathcal{T}_{2\dots m}^* \\ &= \oint \frac{d\zeta^2}{2\pi i \zeta^2} \left\{ \frac{1}{2} \sum_{j=1}^m \frac{\zeta^2 + \theta_j^2}{\zeta^2 - \theta_j^2} \right\} \ln(\rho(\zeta)) \mathcal{T}_{1\dots m}^* + \mathcal{T}_{1\dots m}^* \Omega_2 \\ &= \mathcal{T}_{1\dots m}^* \left\{ \Omega_2 + \sum_{j=1}^m \ln \rho(\theta_j) \right\} \end{aligned}$$

and therefore

$$e^{\Omega_2} \mathcal{T}_{1\dots m}^* = \left(\prod_{j=1}^m \rho(\theta_j) \right) \mathcal{T}_{1\dots m}^* e^{\Omega_2}.$$

If we assume that

$$[\mathbf{t}(\theta), \mathbf{b}^*(\zeta) \mathbf{c}^*(\xi)] = 0 \quad (7.27)$$

we obtain

$$e^{\Omega_2} \mathcal{T}_{1\dots m}^* X = \left(\prod_{j=1}^m \rho(\theta) \right) \mathcal{T}_{1\dots m}^* X .$$

Assuming further that

$$[\mathbf{t}(\theta), \mathbf{b}(\zeta)\mathbf{c}(\xi)] = 0 \quad (7.28)$$

it would follow that

$$[\Omega_1, \Omega_2] = 0 \quad (7.29)$$

and therefore

$$\begin{aligned} & \text{tr}^\alpha \left(e^{\Omega_1 + \Omega_2} \mathbf{t}^*(\theta_1) \dots \mathbf{t}^*(\theta_m) X \right) \\ &= \left(\prod_{j=1}^m \rho(\theta) \right) \text{tr}^\alpha \left(e^{\Omega_0} e^{\tilde{\Omega}} \mathbf{t}^*(\theta_1) \dots \mathbf{t}^*(\theta_m) X \right) \\ &= \left(\prod_{j=1}^m 2\rho(\theta) \right) \text{tr}^\alpha \left(e^{\Omega_0} e^{\tilde{\Omega}} X \right) \end{aligned} \quad (7.30)$$

which is exactly the needed behaviour for Ω_2 . In contrast to [58] we have now derived properties for the operator \mathbf{t} rather than for its modes. Later we will use these properties to derive equations for the modes of \mathbf{t} . We will do this for the inhomogeneous case to be able to compare to [58] and then for the homogeneous case. First however, we shall list all other properties that \mathbf{t} and its modes need to obey.

In contrast to [53], the Ω_2 which is considered here is not nilpotent. In analogy to [58] we shall however require \mathbf{t} to obey a similar property. We assume that \mathbf{t} has the following analytic structure:

$$\mathbf{t}(\zeta) = \sum_{j=0}^{\infty} \frac{\mathbf{t}_j}{(\zeta^2 - 1)^j} . \quad (7.31)$$

Also setting

$$\frac{\ln \rho(\zeta)}{\zeta^2} = \sum_{m=0}^{\infty} \ln \tilde{\rho}_m (\zeta^2 - 1)^m \quad (7.32)$$

we have

$$\begin{aligned} e^{\Omega_2} q^{2\alpha S(0)} X_{[1,l]} &= \exp \left\{ \oint \frac{d\zeta^2}{2\pi i} \sum_{j=0}^{\infty} \sum_{m=0}^{\infty} \frac{\ln \tilde{\rho}_m \mathbf{t}_j}{(\zeta^2 - 1)^{j-m}} \right\} q^{2\alpha S(0)} X_{[1,l]} \\ &= \exp \left\{ \sum_{j=1}^{\infty} \ln \tilde{\rho}_{j-1} \mathbf{t}_j \right\} q^{2\alpha S(0)} X_{[1,l]} . \end{aligned}$$

At this point we require \mathbf{t} to obey the same reduction relations as the other operators:

$$\mathbf{t}_{j,[k,l]} q^{\alpha\sigma_{\tilde{k}}} X_{[k+1,l]} = q^{\alpha\sigma_{\tilde{k}}} \mathbf{t}_{j,[k+1,l]} X_{[k+1,l]}, \quad 1 \leq j \leq l, k < l, \quad (7.33a)$$

$$\mathbf{t}_{j,[1,l]} X_{[1,l-1]} = \mathbf{t}_{j,[1,l-1]} X_{[1,l-1]}, \quad 1 \leq j \leq l, \quad (7.33b)$$

$$\mathbf{t}_{l+1,[1,l+1]} X_{[1,l]} = 0. \quad (7.33c)$$

Note that we require the left reduction only “to the left” of 1. We shall further require that the modes have the projector property

$$\mathbf{t}_j^2 = \mathbf{t}_j, \quad j > 0 \quad (7.34)$$

and that they commute among each other

$$[\mathbf{t}_j, \mathbf{t}_m] = 0, \quad j, m > 0. \quad (7.35)$$

Using these properties, it follows that

$$\begin{aligned} e^{\Omega_2} q^{2\alpha S(0)} X_{[1,l]} &= \prod_{j=1}^l \exp \{ \ln \tilde{\rho}_{j-1} \mathbf{t}_{j,[1,l]} \} q^{2\alpha S(0)} X_{[1,l]} \\ &= \prod_{j=1}^l \{ 1 - \mathbf{t}_{j,[1,l]} + \tilde{\rho}_{j-1} \mathbf{t}_{j,[1,l]} \} q^{2\alpha S(0)} X_{[1,l]} \\ &= \prod_{j=1}^l \{ 1 - \alpha\eta \tilde{\varphi}_{j-1} \mathbf{t}_{j,[1,l]} + \mathcal{O}(\alpha^2) \} q^{2\alpha S(0)} X_{[1,l]} \end{aligned} \quad (7.36)$$

where we have set

$$\tilde{\rho}_j =: 1 - \alpha\eta \tilde{\varphi}_j + \mathcal{O}(\alpha^2). \quad (7.37)$$

We can obtain the $\tilde{\varphi}_j$ from (7.32):

$$\tilde{\varphi}_j = \sum_{k=0}^j \frac{B_1(j,k)}{j!} \varphi^{(k)}, \quad (7.38)$$

where $\varphi^{(k)} = \partial_{\zeta}^k \varphi(\zeta, 0)|_{\zeta=1}$. The $B_1(n, k)$ are given recursively by

$$B_m(0, 0) = 1, \quad (7.39a)$$

$$B_m(n, k) = 0 \quad \text{if } k < 0 \text{ or } k > n, \quad (7.39b)$$

$$B_m(n, k) = \frac{1}{2} B_m(n-1, k-1) - \frac{1}{2} (2n+2m-2-k) B_m(n-1, k) \quad \text{else.} \quad (7.39c)$$

We shall now require that \mathbf{t} is of order $\mathcal{O}(\alpha^{-1})$. This was checked in [58] in the inhomogeneous case for $n = 1, 2, 3$. Going further we will assume this to be true in the homogeneous case and for arbitrary n . Define

$$\mathbf{t}_j^{(0)} = \lim_{\alpha \rightarrow 0} (1 - q^\alpha) \mathbf{t}_j. \quad (7.40)$$

We then have

$$\mathbf{t}_j = -\frac{\mathbf{t}_j^{(0)}}{\alpha\eta} + \mathcal{O}(1). \quad (7.41)$$

It follows that

$$e^{\Omega_2} q^{2\alpha S(0)} X_{[1,l]} = \prod_{j=1}^l \left\{ 1 + \tilde{\varphi}_{j-1} \mathbf{t}_{j,[1,l]}^{(0)} + \mathcal{O}(\alpha) \right\} q^{2\alpha S(0)} X_{[1,l]}. \quad (7.42)$$

We can now consider the case that $X_{[1,l]}$ is even under spin reversal. As we know, the expectation value of such an operator is even in \hbar : $\langle X \rangle_{T,h} = \langle X \rangle_{T,-h}$. Since $\langle X \rangle_{T,h} = \lim_{\alpha \rightarrow 0} \text{tr}^\alpha (e^{\Omega_1 + \Omega_2} X)$, we require $e^{\Omega_2} q^{2\alpha S(0)} X_{[1,l]}$ to be even in \hbar in the limit $\alpha \rightarrow 0$. Since we know that the $\tilde{\varphi}_j$ are odd in \hbar , we know that all products of the $\tilde{\varphi}_j$ with an uneven number of factors have to vanish.

Furthermore, we can observe that

$$\mathbf{t}_i^{(0)} \mathbf{t}_j^{(0)} = 0. \quad (7.43)$$

This was proven in [58] for $n = 1, 2$. Additionally the authors kindly provided us with the data for the $\mathbf{t}_{j,[1,3]}$ with which we were able to verify that the above assumption also holds for $n = 3$. Assuming that this is generally true in the homogeneous case, this means that the $\tilde{\varphi}_j$ only enter the result linearly. It would therefore follow that for an even operator X

$$\lim_{\alpha \rightarrow 0} \text{tr}^\alpha \left(e^{\Omega_2} q^{2\alpha S(0)} X_{[1,l]} \right) = X_{[1,l]}. \quad (7.44)$$

If an operator \mathbf{t} exists, which satisfies all above assumptions, we have then proven that

$$\langle X \rangle_{T,h} = \lim_{\alpha \rightarrow 0} \text{tr}^\alpha (e^{\Omega_1} X), \quad \text{if } \mathbb{J}(X) = X. \quad (7.45)$$

7.3.1 Left Reduction Relation of the Density Matrix

In the above section we have discussed which relations the operator \mathbf{t} needs to obey focusing only on the behaviour of the map $\text{tr}^\alpha (e^{\Omega}(\cdot))$. There is however one additional property that \mathbf{t} needs to obey which follows from the known reduction properties of the density matrix. In [58] the left reduction property of the density matrix is given by

$$\text{tr}_1 \left\{ D_N(\xi_1, \dots, \xi_m | \kappa, \alpha) q^{\alpha \sigma_1^z} \right\} = \rho(\xi_1) D_N(\xi_2, \dots, \xi_m | \kappa, \alpha).$$

In the homogeneous case we would expect D_N to obey the relation

$$\text{tr}_1 \left\{ D_{N,[1,m]}(\kappa, \alpha) q^{\alpha \sigma_1^z} \right\} = \rho(1) D_{N,[2,m]}(\kappa, \alpha). \quad (7.46)$$

This places an additional restriction on \mathbf{t} since we know from [58] that

$$\langle X_{[1,m]} \rangle_{T,h,\alpha} = \lim_{N \rightarrow \infty} \text{tr}_{[1,m]} \{ D_{N,[1,m]}(\kappa, \alpha) X_{[1,m]} \} = \text{tr}^\alpha \left\{ e^\Omega q^{2\alpha S(0)} X_{[1,m]} \right\}. \quad (7.47)$$

We shall now show that (7.46) is true if \mathbf{t} obeys the relations

$$\mathbf{t}_{1,[1,m]} (q^{\alpha\sigma_1^z} X_{[2,m]}) = q^{\alpha\sigma_1^z} X_{[2,m]} \quad (7.48)$$

and

$$\mathbf{t}_{j,[1,m]} (q^{\alpha\sigma_1^z} X_{[2,m]}) = q^{\alpha\sigma_1^z} \mathbf{t}_{j,[2,m]} (X_{[2,m]}) , \quad 1 < j \leq m . \quad (7.49)$$

The second of these relations is expected as it is just the regular left reduction relation. The first is however very surprising.

Setting $X_{[1,m]} = q^{\alpha\sigma_1^z} Y_{[2,m]}$ and using the above relations as well as $\tilde{\rho}_0 = \rho(1)$ we obtain

$$\begin{aligned} & \text{tr}_{[1,m]} \{ D_{N,[1,m]}(\kappa, \alpha) q^{\alpha\sigma_1^z} Y_{[2,m]} \} \\ &= \text{tr}^\alpha \left\{ e^\Omega q^{2\alpha S(0)} q^{\alpha\sigma_1^z} Y_{[2,m]} \right\} \\ &= \text{tr}^\alpha \left\{ q^{2\alpha S(0)} e^{\Omega_{1,[1,m]}} \prod_{j=1}^m (1 - \mathbf{t}_{j,[1,m]} + \tilde{\rho}_{j-1} \mathbf{t}_{j,[1,m]}) q^{\alpha\sigma_1^z} Y_{[2,m]} \right\} \\ &= \text{tr}^\alpha \left\{ q^{2\alpha S(0)} q^{\alpha\sigma_1^z} e^{\Omega_{1,[2,m]}} \tilde{\rho}_0 \prod_{j=2}^m (1 - \mathbf{t}_{j,[2,m]} + \tilde{\rho}_{j-1} \mathbf{t}_{j,[2,m]}) Y_{[2,m]} \right\} \\ &= \tilde{\rho}_0 \text{tr}^\alpha \left\{ q^{2\alpha S(0)} q^{\alpha\sigma_1^z} e^{\Omega_{[2,m]}} Y_{[2,m]} \right\} \\ &= \rho(1) \text{tr}_{[1,m]}^\alpha \left\{ q^{\alpha\sigma_1^z} e^{\Omega_{[2,m]}} Y_{[2,m]} \right\} \\ &= \rho(1) \text{tr}_{[2,m]}^\alpha \left\{ e^{\Omega_{[2,m]}} Y_{[2,m]} \right\} . \end{aligned} \quad (7.50)$$

The reduction relations for \mathbf{t} as well as for Ω_1 were used in the third step. On the other hand consider similarly

$$\begin{aligned} & \text{tr}_{[2,m]} \{ D_{N,[2,m]}(\kappa, \alpha) Y_{[2,m]} \} \\ &= \text{tr}^\alpha \left\{ e^\Omega q^{2\alpha S(1)} Y_{[2,m]} \right\} \\ &= \text{tr}_{[2,m]}^\alpha \left\{ e^{\Omega_{[2,m]}} Y_{[2,m]} \right\} . \end{aligned} \quad (7.51)$$

We now have shown that

$$\begin{aligned} & \text{tr}_{[1,m]} \{ D_{N,[1,m]}(\kappa, \alpha) q^{\alpha\sigma_1^z} Y_{[2,m]} \} = \rho(1) \text{tr}_{[2,m]} \{ D_{N,[2,m]}(\kappa, \alpha) Y_{[2,m]} \} \\ \Rightarrow & \text{tr}_{[2,m]} \left\{ \text{tr}_1 (D_{N,[1,m]}(\kappa, \alpha) q^{\alpha\sigma_1^z}) Y_{[2,m]} \right\} = \rho(1) \text{tr}_{[2,m]} \{ D_{N,[2,m]}(\kappa, \alpha) Y_{[2,m]} \} \\ \Rightarrow & \text{tr}_1 (D_{N,[1,m]}(\kappa, \alpha) q^{\alpha\sigma_1^z}) = \rho(1) D_{N,[2,m]}(\kappa, \alpha) \end{aligned} \quad (7.52)$$

which proves that (7.46) is true if the above reduction relations for \mathbf{t} apply.

The right reduction of the density matrix follows trivially from the right reduction of the \mathbf{t} operator that was already assumed earlier. As such it places no further restrictions on \mathbf{t} .

7.4 Relations for Modes of $\mathbf{t}(\zeta)$

In the above section we explained that the operator \mathbf{t} needs to obey (7.26). Here we will derive the implications of this for the modes of \mathbf{t} . We shall provide the relations and compare them to the ones derived in [58].

7.4.1 Inhomogeneous Case

We will first discuss the inhomogeneous case as this will allow us to verify that (7.26) is compatible with the relations given in [58].

For the sake of readability, we shall write down the three relations derived in [58]:

$$\begin{aligned}\mathbf{t}_j \mathbf{t}_k^* &= \mathbf{t}_j^* \mathbf{t}_k \quad \text{for } j \neq k, \\ \mathbf{t}_j \mathbf{t}_j^* &= \mathbf{t}_j^*, \\ \mathbf{t}_j^* \mathbf{t}_j &= 0.\end{aligned}$$

In the inhomogeneous case the modes of \mathbf{t} are the residues at the places of the inhomogeneities:

$$\mathbf{t}_j = \text{res}_{\zeta=\xi_j} \mathbf{t}(\zeta) \frac{d\zeta^2}{\zeta^2}. \quad (7.53)$$

For the creation operators the modes are the specializations

$$\mathbf{t}_j^* = \mathbf{t}^*(\xi_j). \quad (7.54)$$

We therefore consider the closed integral over (7.26) around ξ_j and set $\theta = \xi_k$:

$$\begin{aligned}\oint_{\xi_j} \frac{d\zeta^2}{2\pi i \zeta^2} (\mathbf{t}(\zeta) \mathbf{t}^*(\xi_k) - \mathbf{t}^*(\xi_k) \mathbf{t}(\zeta)) &= \frac{1}{2} \oint_{\xi_j} \frac{d\zeta^2}{2\pi i \zeta^2} \frac{\zeta^2 + \xi_k^2}{\zeta^2 - \xi_k^2} \mathbf{t}^*(\xi_k) \\ \Rightarrow \mathbf{t}_j \mathbf{t}_k^* - \mathbf{t}_k^* \mathbf{t}_j &= \delta_{jk} \mathbf{t}_k^*,\end{aligned} \quad (7.55)$$

which seems like a contradiction to [58]. To understand that this is actually no contradiction we shall shortly explain the general properties of the creation operators in the inhomogeneous case. For the creation operators $\mathbf{x}^* = \mathbf{t}^*, \mathbf{c}^*, \mathbf{b}^*$ [50] states that if $X_{[k,m]} \in M_{[k,m]}$ and $m < j \leq l$ then $\mathbf{x}_{[k,l]}^*(\zeta, \alpha) X_{[k,m]}$ is regular at $\zeta^2 = \xi_j^2$ and $\mathbf{x}_{[k,l]}^*(\xi_j, \alpha) X_{[k,m]} \in M_{[k,j]}$ is independent of l . Furthermore the inductive limit of $\mathbf{x}_{[k,l]}^*(\xi_j, \alpha) X_{[k,m]}$ is well defined only if $m < j$ which is implied in all relations given in [58].

Given this restriction we know that the first equation from [58] given above is only defined on the subspace $M_{[1,l]}$ with $l < j, k$. On this subspace the right-hand side is always zero because the \mathbf{t}_k obey the annihilation property:

$$\mathbf{t}_j \mathbf{t}_k^* = \mathbf{t}_j^* \mathbf{t}_k = 0, \quad j \neq k. \quad (7.56)$$

Since we do not know the exact behaviour of \mathbf{t} and the paper gives no details about the subspace on which the relations are defined it is conceivable that this equation could be defined for $l < k$ but $l \geq j$. Our tests on the computer show however that the equation is not fulfilled in this case. This leads us to believe that the authors intended to claim this relation only on the smaller subspace $l < j, k$. On this subspace and in the case $j \neq k$ our equation yields the same result. This means that in this case our results are indeed compatible with [58]. An interesting difference is that in contrast to [58] our equation is well defined in the case $l < k$ but $l \geq j$. Using the operator \mathbf{t} which was provided to us by the authors we can verify that this operator does fulfil our equation even in the case $l \geq j$.

Now consider the second and third equations of [58] given above. Our equation (7.55) becomes

$$\mathbf{t}_j \mathbf{t}_j^* - \mathbf{t}_j^* \mathbf{t}_j = \mathbf{t}_j^*$$

and it is clear that this is only well defined on the subspace with $l < j$. On this subspace however the equation simplifies to

$$\mathbf{t}_j \mathbf{t}_j^* = \mathbf{t}_j^*$$

which is the second equation of [58]. The only remaining difference to the paper is now the relation $\mathbf{t}_j^* \mathbf{t}_j = 0$. From our equations it is clear that this property is only needed on the subspace $l < j$ on which this is true because of the annihilation property. We believe that the same restriction applies to [58] although this is never specified explicitly in the paper. Using the data for \mathbf{t} provided to us we verified on the computer that

$$\mathbf{t}_{j,[1,3]}^* \mathbf{t}_{j,[1,3]} X_{[1,l]} = 0, \quad l < j, j = 1, 2, 3$$

as we expected and that

$$\mathbf{t}_{j,[1,3]}^* \mathbf{t}_{j,[1,3]} X_{[1,l]} \neq 0, \quad l = j, j = 1, 2, 3.$$

It is therefore clear that our results are in agreement with [58] even though there seems to be a contradiction at first glance.

7.4.2 Homogeneous Case

To obtain relations for the homogeneous case one needs to insert the appropriate expansions into (7.26). This means the known expansions for \mathbf{t} and \mathbf{t}^* as well as

$$\frac{\zeta^2 + \theta^2}{\zeta^2 - \theta^2} = -1 + 2 \sum_{k=0}^{\infty} \frac{(\theta^2 - 1)^k}{(\zeta^2 - 1)^{k+1}} + 2 \sum_{k=0}^{\infty} \frac{(\theta^2 - 1)^k}{(\zeta^2 - 1)^k}, \quad |1 - \theta^2| < |1 - \zeta^2|.$$

We then obtain

$$2 \sum_{\substack{p=1 \\ j=0}}^{\infty} (\mathbf{t}_j \mathbf{t}_p^* - \mathbf{t}_p^* \mathbf{t}_j) \frac{(\theta^2 - 1)^{p-1}}{(\zeta^2 - 1)^j} =$$

$$- \sum_{m=1}^{\infty} \mathbf{t}_m^* (\theta^2 - 1)^{m-1} + 2 \sum_{\substack{k=0 \\ m=1}}^{\infty} \mathbf{t}_m^* \frac{(\theta^2 - 1)^{k+m-1}}{(\zeta^2 - 1)^{k+1}} + 2 \sum_{\substack{k=0 \\ m=1}}^{\infty} \mathbf{t}_m^* \frac{(\theta^2 - 1)^{k+m-1}}{(\zeta^2 - 1)^k} .$$

From this it follows that the modes \mathbf{t}_j have to obey the following relations:

$$2 (\mathbf{t}_0 \mathbf{t}_p^* - \mathbf{t}_p^* \mathbf{t}_0) = \mathbf{t}_p^* \quad (7.57a)$$

$$\mathbf{t}_j \mathbf{t}_p^* - \mathbf{t}_p^* \mathbf{t}_j = \mathbf{t}_{p-j+1}^* + \mathbf{t}_{p-j}^* \quad , \quad j > 0 \quad , \quad (7.57b)$$

where we have set $\mathbf{t}_p^* = 0$ if $p \leq 0$.

Chapter 8

Conclusion

In this work we used the fermionic structure that was first discovered in [49] to calculate thermal expectation values of the XXZ Heisenberg chain in an external field. We retraced the construction which was expanded in several different papers and added some explanations where we felt that the original literature was unclear. To calculate correlation functions explicitly we constructed all needed fermionic operators for the homogeneous case explicitly on the computer. In order to obtain these, new programs were developed. To our knowledge this has not previously been done for the homogeneous case or for length $n = 5$.

We believe that it would be possible to obtain correlation functions for $n = 6$ using our programs in a reasonable time on moderate hardware. The problems in constructing the fermionic operators for $n = 6$ were already discussed in chapter 5, but we believe they would be solvable given more time. One restriction that would apply to the case $n = 6$ would be the numerical precision of ω . As we explained, errors can be detected but it might be necessary to optimize the C program that calculates ω to obtain correlations for $\Delta > 0.9$.

In addition to the calculations using the exponential form we expressed the operators $\sigma_1^z \sigma_n^z$ and $\sigma_1^x \sigma_n^x$ in terms of the fermionic basis and then used the JMS theorem to obtain the correlation functions. To our knowledge this has not previously been done explicitly. As discussed before this method does not seem feasible for large n , especially compared to the method of the exponential form. However, an open question that should be investigated further is whether it is possible to explicitly express certain operators like e.g. $\sigma_1^z \sigma_n^z$ in terms of the fermionic basis. This could either be a solution to the inverse problem or an asymptotic expression valid for large n . Since the computational difficulties of this approach arise solely in the construction of the operators and the basis transformation, such representations would make it possible to calculate expectation values of the involved operators for large n . We would like to stress that even the explicit construction of the

fermionic operators would become unnecessary if we had a closed expression for certain operators in terms of the fermionic basis. As such we believe that even $n > 10$ would be possible in this scenario. This estimation refers to the algebraic part of the problem. Of course the issue of the numerical precision of ω would still need to be solved like in the case of the exponential form.

We provided a proof for the correctness of the method of the exponential form using the JMS theorem. Although such a proof is in principle already done in [50] our proof is more general as it is valid for finite temperatures and non-vanishing external fields, at least in the case of operators which are even under spin reversal. Our proof still relies on the existence of the operator \mathbf{t} however. Even though a proof of its existence still eludes us, there is strong evidence for it. An open question for future work would be the extension of the proof to the case of an external field and operators not even under spin reversal. It is shown in [57] that the operator \mathbf{h} enters the exponential form of the density matrix in this case. As noted in [58] this operator seems to be connected to \mathbf{t} . We believe that by further investigating this connection it would be possible to generalize our proof. In the end the operator \mathbf{h} would no longer be needed since everything could be expressed in terms of \mathbf{t} . Nevertheless, it may still be practical to use \mathbf{h} since a direct rule for its construction is known which is very similar to the expression for \mathbf{k} . An additional benefit of such a work might be a hint to a possible construction of \mathbf{t} since it is known how to construct \mathbf{h} in general. Another possible approach to further investigate the operator \mathbf{t} would be to use the freedom of choice remaining when choosing Ω_2 in [58]. Choosing this operator differently might lead to a simpler structure of \mathbf{t} .

The calculation of exact and explicit results in a true many-particle system is a rare feat in physics and to our knowledge only possible for integrable models. For this reason we think that the theory of the fermionic basis presented in this work is quite impressive. For the Heisenberg chain it provides us with the knowledge of static short-distance correlations which complements the asymptotic results nicely. As we have shown, asymptotic formulae for low temperatures [72] allow the calculation of correlation functions for $n \geq 5$ to a very reasonable precision. At the same time it seems realistic to derive asymptotics for the high-temperature case. The case of the massive regime was not explicitly covered in this work. However, the algebraic part of the construction, which was the focus of our work, does not depend on physical parameters. As such, to calculate expectation values for the massive regime, one would only need to obtain the function ω for this case. The rest of the procedure would remain the same. A program for the massive case has already been created by Trippe and Damerau [73]. In this case, the experience is that the numerics are easier. This is likely because the integration contours are finite in both directions, resulting in finite integrals in the NLIEs. As in the massless case, there are asymptotic formulae which are close to the exact results for relatively small n . These were derived in [74, 75]. Here the

authors derived form factor series representations of the two-point correlation functions in the ground state. These are obtained using the algebraic Bethe ansatz applied to the ordinary and the quantum transfer matrix respectively.

As explained before, short-distance static correlation functions can also be observed experimentally, e.g. in electron spin resonance (ESR) experiments. Using linear response theory, the moments of absorption lines can be related to short-distance static correlations [19, 20]. In [23] the authors used the compound $\text{Cu}(\text{py})_2\text{Br}_2$ in ESR experiments and found a good agreement with the next-nearest neighbour functions. Since longer distances relate to higher moments of absorption lines, correlation functions become difficult to measure. One simple reason for this is that the “tails” of the absorption lines become difficult to measure due to a low signal-to-noise ratio. This experimental difficulty, among others, is discussed in the paper. However, measurements for longer distances may become possible in the future as experimental methods improve.

We would also like to mention that there are recent works on the calculation of short-distance static correlations for the Heisenberg chain. These are of special interest to us because they make use of the construction of the fermionic basis as well. In [76] the authors developed a method to “guess” the coefficients of an expansion of quasi-local operators into a sum of products of creation operators. This method is similar to the operator product expansion (OPE) of quantum field theory and makes use of the fact that the theory developed in [52] is valid for arbitrary Matsubara data (see section 4.1), i.e. spectral parameters and choice of representations on the horizontal lines. The idea is that the algebraic part does not depend on the choice of the Matsubara data which fixes the physical parameters. It is therefore possible to choose the Matsubara data in such a way that one- and two-point functions can be easily calculated. The OPE can then be fixed by considering the expectation values of an operator and its expansion. The so-obtained expansion can then be used with other data corresponding to a physical case. This method allows to perform computations for up to 11 sites, but is only performed for the XXX case. In [77] the method is expanded to obtain the entire density matrix of the XXX chain for up to 10 sites, but with the restriction of \mathfrak{sl}_2 invariance, i.e. in the absence of an external field. In [78] the method was then applied to calculate the density matrix of the XXZ chain for up to 8 sites, however only for the case of an unbroken $U_q(\mathfrak{sl}_2)$ symmetry. Even though the author is able to do computations for larger intervals than we are, the restriction to $U_q(\mathfrak{sl}_2)$ symmetry is a very strong one. It restricts the author to the case of a vanishing external field and also forbids the calculation of two-point functions which we are interested in. In [79] the authors prove that for operators invariant under $U_q(\mathfrak{sl}_2)$ the correlation functions do not contain the function ω' . For this reason it follows that none of the correlation functions calculated in our work are accessible through the OPE technique. As the author states, it would be complicated to remove this restriction.

We believe that in the case of broken symmetry it would not be possible to obtain results for 8 sites since all expressions would become significantly more complicated. The main reason that the author did not expand the method is probably that his interest is focused on CFT. Unbroken quantum group symmetry corresponds to a fixed twist q^{-S} which corresponds to a central charge of $c = 1 - 6\nu^2/(1 - \nu)$ in the scaling limit rather than $c = 1$. Since we are more interested in the lattice model, we are naturally interested in the case of broken quantum group symmetry, too. As such it seems to be unclear whether the method of OPE is superior to the method of the exponential form, although it would be interesting to develop it further. An additional advantage of our method might be that we already computed all fermionic operators for arbitrary spin. In our case we concentrate on the spin zero sector but, using the fermionic basis, it would be possible to calculate other contributions and with them objects like form factors.

In the end we think that the study of the fermionic basis is interesting not only to obtain measurable quantities like correlation functions but also to enhance our understanding of the structure of the Heisenberg model or even integrable models in general. An interesting question in this context could be if it is possible to obtain the construction of the fermionic basis directly from the appropriate quantum groups, like $U_q(\widehat{\mathfrak{sl}}_2)$ in our example. Such connections would extend our general understanding and might allow us to develop much more efficient methods for the calculation of static correlation functions of integrable spin chains.

$$\begin{aligned}
& b_3^* t_1^* t_3^* - b_4^* t_1^* t_2^* , \quad c_1^* b_1^* t_1^* t_4^* - c_1^* b_1^* t_2^* t_3^* + c_2^* b_1^* (t_2^*)^2 - c_2^* b_2^* t_1^* t_2^* - c_3^* b_1^* t_1^* t_2^* + \\
& c_3^* b_2^* (t_1^*)^2 - b_3^* c_1^* t_1^* t_2^* + b_4^* c_1^* (t_1^*)^2 , \quad b_1^* t_1^* t_4^* - b_1^* t_2^* t_3^* + b_3^* t_1^* t_2^* - b_4^* (t_1^*)^2 , \\
& c_1^* b_1^* t_1^* t_3^* - c_1^* b_1^* (t_2^*)^2 + c_2^* b_1^* t_1^* t_2^* - c_3^* b_1^* (t_1^*)^2 , \quad b_1^* t_1^* t_3^* - b_1^* (t_2^*)^2 , \quad c_1^* (t_1^*)^2 t_3^* - \\
& c_1^* t_1^* (t_2^*)^2 + c_2^* (t_1^*)^2 t_2^* - c_3^* (t_1^*)^3 , \quad (t_1^*)^2 t_3^* - t_1^* (t_2^*)^2 , \quad c_2^* b_3^* b_2^* b_1^* + b_4^* c_1^* b_2^* b_1^* , \\
& b_4^* b_2^* b_1^* , \quad c_1^* b_2^* b_1^* t_4^* - c_2^* b_2^* b_1^* t_3^* + c_2^* b_3^* b_1^* t_2^* - c_2^* b_3^* b_2^* t_1^* + b_4^* c_1^* b_1^* t_2^* - b_4^* c_1^* b_2^* t_1^* \\
& , \quad b_2^* b_1^* t_4^* - b_4^* b_1^* t_2^* + b_4^* b_2^* t_1^* , \quad c_1^* b_2^* b_1^* t_3^* - c_2^* b_2^* b_1^* t_2^* + c_2^* b_3^* b_1^* t_1^* + b_4^* c_1^* b_1^* t_1^* , \\
& b_2^* b_1^* t_3^* - b_4^* b_1^* t_1^* , \quad c_1^* b_2^* b_1^* t_2^* - c_2^* b_2^* b_1^* t_1^* , \quad b_2^* b_1^* t_2^* , \quad c_1^* b_1^* t_1^* t_4^* - c_1^* b_1^* t_2^* t_3^* + \\
& c_1^* b_2^* t_1^* t_3^* - c_2^* b_1^* t_1^* t_3^* + c_2^* b_1^* (t_2^*)^2 - c_2^* b_2^* t_1^* t_2^* + c_2^* b_3^* (t_1^*)^2 + b_4^* c_1^* (t_1^*)^2 , \\
& b_1^* t_1^* t_4^* - b_1^* t_2^* t_3^* + b_2^* t_1^* t_3^* - b_4^* (t_1^*)^2 , \quad c_1^* b_1^* (t_2^*)^2 - c_1^* b_2^* t_1^* t_2^* - c_2^* b_1^* t_1^* t_2^* + \\
& c_2^* b_2^* (t_1^*)^2 , \quad b_1^* (t_2^*)^2 - b_2^* t_1^* t_2^* , \quad c_1^* b_1^* t_1^* t_2^* - c_2^* b_1^* (t_1^*)^2 , \quad b_1^* t_1^* t_2^* , \quad c_1^* (t_1^*)^2 t_2^* - \\
& c_2^* (t_1^*)^3 , \quad (t_1^*)^2 t_2^* , \quad c_1^* b_3^* b_2^* b_1^* , \quad b_3^* b_2^* b_1^* , \quad c_1^* b_2^* b_1^* t_3^* - c_1^* b_3^* b_1^* t_2^* + c_1^* b_3^* b_2^* t_1^* \\
& , \quad b_2^* b_1^* t_3^* - b_3^* b_1^* t_2^* + b_3^* b_2^* t_1^* , \quad c_1^* b_2^* b_1^* t_2^* - c_1^* b_3^* b_1^* t_1^* , \quad b_2^* b_1^* t_2^* - b_3^* b_1^* t_1^* \\
& , \quad c_1^* b_2^* b_1^* t_1^* , \quad b_2^* b_1^* t_1^* , \quad c_1^* b_1^* t_1^* t_3^* - c_1^* b_1^* (t_2^*)^2 + c_1^* b_2^* t_1^* t_2^* - c_1^* b_3^* (t_1^*)^2 , \\
& b_1^* t_1^* t_3^* - b_1^* (t_2^*)^2 + b_2^* t_1^* t_2^* - b_3^* (t_1^*)^2 , \quad c_1^* b_1^* t_1^* t_2^* - c_1^* b_2^* (t_1^*)^2 , \quad b_1^* t_1^* t_2^* - \\
& b_2^* (t_1^*)^2 , \quad c_1^* b_1^* (t_1^*)^2 , \quad b_1^* (t_1^*)^2 , \quad c_1^* (t_1^*)^3 , \quad (t_1^*)^3 , \quad c_4^* c_3^* b_2^* b_1^* + c_4^* b_3^* c_2^* b_1^* + \\
& c_4^* b_3^* b_2^* c_1^* + b_4^* c_3^* c_2^* b_1^* + b_4^* c_3^* b_2^* c_1^* + b_4^* b_3^* c_2^* c_1^* , \quad c_4^* b_3^* b_2^* + b_4^* c_3^* b_2^* + b_4^* b_3^* c_2^* \\
& , \quad c_4^* b_3^* b_1^* + b_4^* c_3^* b_1^* + b_4^* b_3^* c_1^* , \quad b_4^* b_3^* , \quad c_3^* c_2^* b_1^* t_4^* + c_3^* b_2^* c_1^* t_4^* - c_4^* c_2^* b_1^* t_3^* + \\
& c_4^* c_3^* b_1^* t_2^* - c_4^* c_3^* b_2^* t_1^* - c_4^* b_2^* c_1^* t_3^* + c_4^* b_3^* c_1^* t_2^* - c_4^* b_3^* c_2^* t_1^* + b_3^* c_2^* c_1^* t_4^* - b_4^* c_2^* c_1^* t_3^* + \\
& b_4^* c_3^* c_1^* t_2^* - b_4^* c_3^* c_2^* t_1^* , \quad c_3^* b_2^* t_4^* - c_4^* b_2^* t_3^* + c_4^* b_3^* t_2^* + b_3^* c_2^* t_4^* - b_4^* c_2^* t_3^* + b_4^* c_3^* t_2^* \\
& , \quad c_3^* b_1^* t_4^* - c_4^* b_1^* t_3^* + c_4^* b_3^* t_1^* + b_3^* c_1^* t_4^* - b_4^* c_1^* t_3^* + b_4^* c_3^* t_1^* , \quad b_3^* t_4^* - b_4^* t_3^* \\
& , \quad c_3^* c_2^* b_1^* t_3^* + c_3^* b_2^* c_1^* t_3^* - c_4^* c_2^* b_1^* t_2^* + c_4^* c_3^* b_1^* t_1^* - c_4^* b_2^* c_1^* t_2^* + c_4^* b_3^* c_1^* t_1^* + \\
& b_3^* c_2^* c_1^* t_3^* - b_4^* c_2^* c_1^* t_2^* + b_4^* c_3^* c_1^* t_1^* , \quad c_3^* b_2^* t_3^* - c_4^* b_2^* t_2^* + c_4^* b_3^* t_1^* + b_3^* c_2^* t_3^* - \\
& b_4^* c_2^* t_2^* + b_4^* c_3^* t_1^* , \quad c_3^* b_1^* t_3^* - c_4^* b_1^* t_2^* + b_3^* c_1^* t_3^* - b_4^* c_1^* t_2^* , \quad b_3^* t_3^* - b_4^* t_2^* \\
& , \quad c_2^* c_1^* t_2^* t_4^* - c_2^* c_1^* (t_3^*)^2 - c_3^* c_1^* t_1^* t_4^* + c_3^* c_1^* t_2^* t_3^* - c_3^* c_2^* t_1^* t_3^* + c_4^* c_1^* t_1^* t_3^* - \\
& c_4^* c_1^* (t_2^*)^2 + c_4^* c_2^* t_1^* t_2^* - c_4^* c_3^* (t_1^*)^2 , \quad c_2^* t_2^* t_4^* - c_2^* (t_3^*)^2 - c_3^* t_1^* t_4^* + c_3^* t_2^* t_3^* + \\
& c_4^* t_1^* t_3^* - c_4^* (t_2^*)^2 , \quad c_1^* t_2^* t_4^* - c_1^* (t_3^*)^2 + c_3^* t_1^* t_3^* - c_4^* t_1^* t_2^* , \quad t_2^* t_4^* - (t_3^*)^2 , \\
& c_3^* b_3^* c_2^* b_1^* + c_3^* b_3^* b_2^* c_1^* + c_4^* c_2^* b_2^* b_1^* + c_4^* b_3^* c_1^* b_1^* + b_4^* c_2^* b_2^* c_1^* + b_4^* c_3^* c_1^* b_1^* , \\
& c_3^* b_3^* b_2^* - c_4^* b_3^* b_1^* + b_4^* c_2^* b_2^* - b_4^* c_3^* b_1^* , \quad c_3^* b_3^* b_1^* - c_4^* b_2^* b_1^* - b_4^* b_2^* c_1^* , \quad b_4^* b_2^* \\
& , \quad c_2^* b_2^* c_1^* t_4^* + c_3^* c_1^* b_1^* t_4^* - c_3^* c_2^* b_1^* t_3^* - c_3^* b_2^* c_1^* t_3^* + c_3^* b_3^* c_1^* t_2^* - c_3^* b_3^* c_2^* t_1^* - \\
& c_4^* c_1^* b_1^* t_3^* + c_4^* c_2^* b_1^* t_2^* - c_4^* c_2^* b_2^* t_1^* - c_4^* b_3^* c_1^* t_1^* + b_4^* c_2^* c_1^* t_2^* - b_4^* c_3^* c_1^* t_1^* , \quad c_2^* b_2^* t_4^* - \\
& c_3^* b_1^* t_4^* - c_3^* b_2^* t_3^* + c_3^* b_3^* t_2^* + c_4^* b_1^* t_3^* - c_4^* b_3^* t_1^* + b_4^* c_2^* t_2^* - b_4^* c_3^* t_1^* , \quad c_3^* b_1^* t_3^* - \\
& c_3^* b_3^* t_1^* - c_4^* b_1^* t_2^* + c_4^* b_2^* t_1^* + b_2^* c_1^* t_4^* - b_4^* c_1^* t_2^* , \quad b_2^* t_4^* - b_4^* t_2^* , \quad c_2^* b_2^* c_1^* t_3^* + \\
& c_3^* c_1^* b_1^* t_3^* - c_3^* c_2^* b_1^* t_2^* - c_3^* b_2^* c_1^* t_2^* + c_3^* b_3^* c_1^* t_1^* - c_4^* c_1^* b_1^* t_2^* + c_4^* c_2^* b_1^* t_1^* + b_4^* c_2^* c_1^* t_1^* \\
& , \quad c_2^* b_2^* t_3^* - c_3^* b_1^* t_3^* - c_3^* b_2^* t_2^* + c_3^* b_3^* t_1^* + c_4^* b_1^* t_2^* + b_4^* c_2^* t_1^* , \quad c_3^* b_1^* t_2^* - c_4^* b_1^* t_1^* + \\
& b_2^* c_1^* t_3^* - b_4^* c_1^* t_1^* , \quad b_2^* t_3^* - b_4^* t_1^* , \quad c_2^* c_1^* t_1^* t_4^* - c_2^* c_1^* t_2^* t_3^* + c_3^* c_1^* (t_2^*)^2 - c_3^* c_2^* t_1^* t_2^* - \\
& c_4^* c_1^* t_1^* t_2^* + c_4^* c_2^* (t_1^*)^2 , \quad c_2^* t_1^* t_4^* - c_2^* t_2^* t_3^* + c_3^* (t_2^*)^2 - c_4^* t_1^* t_2^* , \quad c_1^* t_1^* t_4^* - \\
& c_1^* t_2^* t_3^* + c_3^* t_1^* t_2^* - c_4^* (t_1^*)^2 , \quad t_1^* t_4^* - t_2^* t_3^* , \quad c_2^* b_3^* b_2^* c_1^* + c_3^* b_3^* c_1^* b_1^* + c_4^* c_1^* b_2^* b_1^* \\
& , \quad c_2^* b_3^* b_2^* - c_3^* b_3^* b_1^* + c_4^* b_2^* b_1^* , \quad b_3^* b_2^* c_1^* , \quad b_3^* b_2^* , \quad c_2^* b_2^* c_1^* t_3^* - c_2^* b_3^* c_1^* t_2^* + \\
& c_3^* c_1^* b_1^* t_3^* + c_3^* b_3^* c_1^* t_1^* - c_4^* c_1^* b_1^* t_2^* + c_4^* c_1^* b_2^* t_1^* , \quad c_2^* b_2^* t_3^* - c_2^* b_3^* t_2^* - c_3^* b_1^* t_3^* + \\
& c_3^* b_3^* t_1^* + c_4^* b_1^* t_2^* - c_4^* b_2^* t_1^* , \quad b_2^* c_1^* t_3^* - b_3^* c_1^* t_2^* , \quad b_2^* t_3^* - b_3^* t_2^* , \quad c_2^* b_2^* c_1^* t_2^* - \\
& c_2^* b_3^* c_1^* t_1^* + c_3^* c_1^* b_1^* t_2^* - c_4^* c_1^* b_1^* t_1^* , \quad c_2^* b_2^* t_2^* - c_2^* b_3^* t_1^* - c_3^* b_1^* t_2^* + c_4^* b_1^* t_1^* , \\
& b_2^* c_1^* t_2^* - b_3^* c_1^* t_1^* , \quad b_2^* t_2^* - b_3^* t_1^* , \quad c_2^* c_1^* t_1^* t_3^* - c_2^* c_1^* (t_2^*)^2 + c_3^* c_1^* t_1^* t_2^* - c_4^* c_1^* (t_1^*)^2 \\
& , \quad c_2^* t_1^* t_3^* - c_2^* (t_2^*)^2 + c_3^* t_1^* t_2^* - c_4^* (t_1^*)^2 , \quad c_1^* t_1^* t_3^* - c_1^* (t_2^*)^2 , \quad t_1^* t_3^* - (t_2^*)^2 , \\
& c_3^* c_2^* b_2^* b_1^* + c_3^* b_3^* c_1^* b_1^* + b_4^* c_2^* c_1^* b_1^* , \quad c_3^* b_3^* b_1^* + b_4^* c_2^* b_1^* , \quad c_3^* b_2^* b_1^* + b_4^* c_1^* b_1^* ,
\end{aligned}$$

$$\begin{aligned}
& b_4^* b_1^*, c_2^* c_1^* b_1^* t_4^* - c_3^* c_1^* b_1^* t_3^* + c_3^* c_2^* b_1^* t_2^* - c_3^* c_2^* b_2^* t_1^* - c_3^* b_3^* c_1^* t_1^* - b_4^* c_2^* c_1^* t_1^* \\
& , c_2^* b_1^* t_4^* - c_3^* b_1^* t_3^* + c_3^* b_3^* t_1^* + b_4^* c_2^* t_1^* , c_1^* b_1^* t_4^* - c_3^* b_1^* t_2^* + c_3^* b_2^* t_1^* + b_4^* c_1^* t_1^* \\
& , b_1^* t_4^* - b_4^* t_1^* , c_2^* c_1^* b_1^* t_3^* - c_3^* c_1^* b_1^* t_2^* + c_3^* c_2^* b_1^* t_1^* , c_2^* b_1^* t_3^* - c_3^* b_1^* t_2^* , \\
& c_1^* b_1^* t_3^* - c_3^* b_1^* t_1^* , b_1^* t_3^* , c_2^* c_1^* t_1^* t_3^* - c_3^* c_1^* t_1^* t_2^* + c_3^* c_2^* (t_1^*)^2 , c_2^* t_1^* t_3^* - c_3^* t_1^* t_2^* , \\
& c_1^* t_1^* t_3^* - c_3^* (t_1^*)^2 , t_1^* t_3^* , c_2^* b_3^* c_1^* b_1^* + c_3^* c_1^* b_2^* b_1^* , c_2^* b_3^* b_1^* - c_3^* b_2^* b_1^* , b_3^* c_1^* b_1^* \\
& , b_3^* b_1^* , c_2^* c_1^* b_1^* t_3^* + c_2^* b_3^* c_1^* t_1^* - c_3^* c_1^* b_1^* t_2^* + c_3^* c_1^* b_2^* t_1^* , c_2^* b_1^* t_3^* - c_2^* b_3^* t_1^* - \\
& c_3^* b_1^* t_2^* + c_3^* b_2^* t_1^* , c_1^* b_1^* t_3^* + b_3^* c_1^* t_1^* , b_1^* t_3^* - b_3^* t_1^* , c_2^* c_1^* b_1^* t_2^* - c_3^* c_1^* b_1^* t_1^* , \\
& c_2^* b_1^* t_2^* - c_3^* b_1^* t_1^* , c_1^* b_1^* t_2^* , b_1^* t_2^* , c_2^* c_1^* t_1^* t_2^* - c_3^* c_1^* (t_1^*)^2 , c_2^* t_1^* t_2^* - c_3^* (t_1^*)^2 , \\
& c_1^* t_1^* t_2^* , t_1^* t_2^* , c_2^* c_1^* b_2^* b_1^* , c_2^* b_2^* b_1^* , c_1^* b_3^* b_1^* , b_2^* b_1^* , c_2^* c_1^* b_1^* t_2^* - c_2^* c_1^* b_2^* t_1^* \\
& , c_2^* b_1^* t_2^* - c_2^* b_2^* t_1^* , c_1^* b_1^* t_2^* - c_1^* b_2^* t_1^* , b_1^* t_2^* - b_2^* t_1^* , c_2^* c_1^* b_1^* t_1^* , c_2^* b_1^* t_1^* , \\
& c_1^* b_1^* t_1^* , b_1^* t_1^* , c_2^* c_1^* (t_1^*)^2 , c_2^* (t_1^*)^2 , c_1^* (t_1^*)^2 , (t_1^*)^2 , c_4^* c_3^* c_2^* b_1^* + c_4^* c_3^* b_2^* c_1^* + \\
& c_4^* b_3^* c_2^* c_1^* + b_4^* c_3^* c_2^* c_1^* , c_4^* c_3^* b_2^* + c_4^* b_3^* c_2^* + b_4^* c_3^* c_2^* , c_4^* c_3^* b_1^* + c_4^* b_3^* c_1^* + b_4^* c_3^* c_1^* \\
& , c_4^* c_2^* b_1^* + c_4^* b_2^* c_1^* + b_4^* c_2^* c_1^* , c_4^* b_3^* + b_4^* c_3^* , c_4^* b_2^* + b_4^* c_2^* , c_4^* b_1^* + b_4^* c_1^* , \\
& b_4^* , c_3^* c_2^* c_1^* t_4^* - c_4^* c_2^* c_1^* t_3^* + c_4^* c_3^* c_1^* t_2^* - c_4^* c_3^* c_2^* t_1^* , c_3^* c_2^* t_4^* - c_4^* c_2^* t_3^* + c_4^* c_3^* t_2^* , \\
& c_3^* c_1^* t_4^* - c_4^* c_1^* t_3^* + c_4^* c_3^* t_1^* , c_2^* c_1^* t_4^* - c_4^* c_1^* t_2^* + c_4^* c_2^* t_1^* , c_3^* t_4^* - c_4^* t_3^* , c_2^* t_4^* - c_4^* t_2^* , \\
& c_1^* t_4^* - c_4^* t_1^* , t_4^* , c_3^* b_3^* c_2^* c_1^* + c_4^* c_2^* b_2^* c_1^* + c_4^* c_3^* c_1^* b_1^* , c_3^* b_3^* c_2^* + c_4^* c_2^* b_2^* - c_4^* c_3^* b_1^* \\
& , c_3^* b_3^* c_1^* - c_4^* b_2^* c_1^* , c_4^* c_1^* b_1^* - b_3^* c_2^* c_1^* , c_3^* b_3^* - c_4^* b_2^* , c_4^* b_1^* + b_3^* c_2^* , b_3^* c_1^* , b_3^* \\
& , c_3^* c_2^* c_1^* t_3^* - c_4^* c_2^* c_1^* t_2^* + c_4^* c_3^* c_1^* t_1^* , c_3^* c_2^* t_3^* - c_4^* c_2^* t_2^* + c_4^* c_3^* t_1^* , c_3^* c_1^* t_3^* - c_4^* c_1^* t_2^* , \\
& c_2^* c_1^* t_3^* - c_4^* c_1^* t_1^* , c_3^* t_3^* - c_4^* t_2^* , c_2^* t_3^* - c_4^* t_1^* , c_1^* t_3^* , t_3^* , c_3^* c_2^* b_2^* c_1^* + c_4^* c_2^* c_1^* b_1^* \\
& , c_3^* c_2^* b_2^* - c_4^* c_2^* b_1^* , c_3^* b_2^* c_1^* + c_4^* c_1^* b_1^* , c_2^* b_2^* c_1^* , c_3^* b_2^* - c_4^* b_1^* , c_2^* b_2^* , b_2^* c_1^* \\
& , b_2^* , c_3^* c_2^* c_1^* t_2^* - c_4^* c_2^* c_1^* t_1^* , c_3^* c_2^* t_2^* - c_4^* c_2^* t_1^* , c_3^* c_1^* t_2^* - c_4^* c_1^* t_1^* , c_2^* c_1^* t_2^* \\
& , c_3^* t_2^* - c_4^* t_1^* , c_2^* t_2^* , c_1^* t_2^* , t_2^* , c_3^* c_2^* c_1^* b_1^* , c_3^* c_2^* b_1^* , c_3^* c_1^* b_1^* , c_2^* c_1^* b_1^* \\
& , c_3^* b_1^* , c_2^* b_1^* , c_1^* b_1^* , b_1^* , c_3^* c_2^* c_1^* t_1^* , c_3^* c_2^* t_1^* , c_3^* c_1^* t_1^* , c_2^* c_1^* t_1^* , c_3^* t_1^* , \\
& c_2^* t_1^* , c_1^* t_1^* , t_1^* , c_4^* c_3^* c_2^* c_1^* , c_4^* c_3^* c_2^* , c_4^* c_3^* c_1^* , c_4^* c_2^* c_1^* , c_3^* c_2^* c_1^* , c_4^* c_3^* , \\
& c_4^* c_2^* , c_3^* c_2^* , c_4^* c_1^* , c_3^* c_1^* , c_2^* c_1^* , c_4^* , c_3^* , c_2^* , c_1^* , 1 .
\end{aligned}$$

Appendix B

Correlation Functions for $n = 5$

In the following we choose to set $\omega_{ij} = \partial_\lambda^i \partial_\mu^j \tilde{\omega}(\lambda, \mu)_{\lambda=\mu=0}$ to shorten the expressions.

$$\begin{aligned} \langle \sigma_1^z \sigma_5^z \rangle = & \\ & \{-8\eta^2 q^2 \{112\omega_{11}\omega_{20} - 112\omega_{10}\omega_{21} - 120\omega_{21}^2 + 120\omega_{11}\omega_{22} + 40\omega_{21}\omega_{30} + 12\omega_{22}\omega_{31} \\ & - 8\omega_{31}^2 - 40\omega_{10}\omega_{32} - 12\omega_{21}\omega_{32} + 4\omega_{30}\omega_{32} + 8\omega_{11}\omega_{33} - 4\omega_{20}\omega_{33} \\ & - 20\omega_{11}\omega_{40} - 3\omega_{22}\omega_{40} + 2\omega_{31}\omega_{40} + 20\omega_{10}\omega_{41} + 6\omega_{21}\omega_{41} - 2\omega_{30}\omega_{41} \\ & - 32q^{14} (9216\omega + 18112\omega_{11} - 12864\omega_{20} - 3084\omega_{22} + 3016\omega_{31} + 148\omega_{33} - 240\omega_{40} - 111\omega_{42}) \\ & - 6\omega_{11}\omega_{42} + 3\omega_{20}\omega_{42} \\ & + q^{18} (-51200\omega_{10}^2 + 25600\omega_{11} - 9216\omega_{20} - 233488\omega_{11}\omega_{20} + 155136\omega_{20}^2 - 15288\omega_{21}^2 \\ & + 14016\omega_{22} + 15288\omega_{11}\omega_{22} + 11240\omega_{21}\omega_{30} - 2048\omega_{30}^2 - 18560\omega_{31} - 6144\omega_{20}\omega_{31} \\ & - 1236\omega_{22}\omega_{31} + 824\omega_{31}^2 + 1236\omega_{21}\omega_{32} - 412\omega_{30}\omega_{32} - 1856\omega_{33} - 824\omega_{11}\omega_{33} \\ & + 412\omega_{20}\omega_{33} + 2304\omega_{40} - 2548\omega_{11}\omega_{40} + 1536\omega_{20}\omega_{40} + 309\omega_{22}\omega_{40} - 206\omega_{31}\omega_{40} \\ & - 618\omega_{21}\omega_{41} + 206\omega_{30}\omega_{41} + 4\omega_{10} (58372\omega_{21} - 25856\omega_{30} + 637(-2\omega_{32} + \omega_{41})) \\ & + 512\omega (-864 + 100\omega_{11} - 303\omega_{22} + 202\omega_{31} + 4\omega_{33} - 3\omega_{42}) \\ & + 1392\omega_{42} + 618\omega_{11}\omega_{42} - 309\omega_{20}\omega_{42}) \\ & + q^{12} (-456704\omega_{10}^2 + 151552\omega_{11} - 142848\omega_{20} - 77136\omega_{11}\omega_{20} + 81408\omega_{20}^2 \\ & - 16920\omega_{21}^2 - 69504\omega_{22} + 16920\omega_{11}\omega_{22} + 21000\omega_{21}\omega_{30} - 5120\omega_{30}^2 + 69376\omega_{31} \\ & - 15360\omega_{20}\omega_{31} - 900\omega_{22}\omega_{31} + 600\omega_{31}^2 + 900\omega_{21}\omega_{32} - 300\omega_{30}\omega_{32} + 3712\omega_{33} \\ & - 600\omega_{11}\omega_{33} + 300\omega_{20}\omega_{33} - 5760\omega_{40} - 2820\omega_{11}\omega_{40} + 3840\omega_{20}\omega_{40} + 225\omega_{22}\omega_{40} \\ & - 150\omega_{31}\omega_{40} - 450\omega_{21}\omega_{41} + 150\omega_{30}\omega_{41} + 4\omega_{10} (19284\omega_{21} - 13568\omega_{30} + 705(-2\omega_{32} + \omega_{41})) \\ & + 256\omega (-2880 + 1784\omega_{11} - 318\omega_{22} + 212\omega_{31} + 20\omega_{33} - 15\omega_{42}) \\ & - 2784\omega_{42} + 450\omega_{11}\omega_{42} - 225\omega_{20}\omega_{42}) \end{aligned}$$

$$\begin{aligned}
& + q^4 (7168\omega_{10}^2 - 7296\omega_{20}^2 + 840\omega_{21}^2 - 576\omega_{22} + 7296\omega\omega_{22} - 2200\omega_{21}\omega_{30} \\
& + 640\omega_{30}^2 + 384\omega_{31} - 4864\omega\omega_{31} + 1920\omega_{20}\omega_{31} - 84\omega_{22}\omega_{31} + 56\omega_{31}^2 \\
& + 84\omega_{21}\omega_{32} - 28\omega_{30}\omega_{32} - 192\omega_{33} - 640\omega\omega_{33} + 28\omega_{20}\omega_{33} - 480\omega_{20}\omega_{40} \\
& + 21\omega_{22}\omega_{40} - 14\omega_{31}\omega_{40} - 42\omega_{21}\omega_{41} + 14\omega_{30}\omega_{41} \\
& - 4\omega_{10} (3932\omega_{21} - 1216\omega_{30} - 70\omega_{32} + 35\omega_{41}) \\
& - 2\omega_{11} (-768 + 3584\omega - 7864\omega_{20} + 420\omega_{22} + 28\omega_{33} - 70\omega_{40} - 21\omega_{42}) \\
& + 144\omega_{42} + 480\omega\omega_{42} - 21\omega_{20}\omega_{42}) \\
& + q^{28} (120\omega_{21}^2 - 40\omega_{21}\omega_{30} - 12\omega_{22}\omega_{31} + 8\omega_{31}^2 + 12\omega_{21}\omega_{32} - 4\omega_{30}\omega_{32} \\
& + 4\omega_{20}\omega_{33} + 3\omega_{22}\omega_{40} - 2\omega_{31}\omega_{40} + 4\omega_{10} (28\omega_{21} + 10\omega_{32} - 5\omega_{41}) \\
& - 6\omega_{21}\omega_{41} + 2\omega_{30}\omega_{41} - 2\omega_{11} (56\omega_{20} + 60\omega_{22} + 4\omega_{33} - 10\omega_{40} - 3\omega_{42}) \\
& - 3\omega_{20}\omega_{42}) \\
& + 8q^6 (2176\omega_{10}^2 - 1968\omega_{20}^2 - 228\omega_{21}^2 - 120\omega_{22} + 1968\omega\omega_{22} - 260\omega_{21}\omega_{30} \\
& + 112\omega_{30}^2 + 80\omega_{31} - 1312\omega\omega_{31} + 336\omega_{20}\omega_{31} + 12\omega_{22}\omega_{31} - 8\omega_{31}^2 - 12\omega_{21}\omega_{32} \\
& + 4\omega_{30}\omega_{32} + 8\omega_{33} - 112\omega\omega_{33} - 4\omega_{20}\omega_{33} - 84\omega_{20}\omega_{40} - 3\omega_{22}\omega_{40} \\
& + 2\omega_{31}\omega_{40} + 6\omega_{21}\omega_{41} - 2\omega_{30}\omega_{41} \\
& + \omega_{10} (-4168\omega_{21} + 1312\omega_{30} - 76\omega_{32} + 38\omega_{41}) \\
& + \omega_{11} (128 - 2176\omega + 4168\omega_{20} + 228\omega_{22} + 8\omega_{33} - 38\omega_{40} - 6\omega_{42}) \\
& - 6\omega_{42} + 84\omega\omega_{42} + 3\omega_{20}\omega_{42}) \\
& + q^2 (4096\omega_{10}^2 - 3840\omega_{20}^2 + 216\omega_{21}^2 - 960\omega_{22} + 3840\omega\omega_{22} - 840\omega_{21}\omega_{30} + 256\omega_{30}^2 \\
& + 640\omega_{31} - 2560\omega\omega_{31} + 768\omega_{20}\omega_{31} + 36\omega_{22}\omega_{31} - 24\omega_{31}^2 - 36\omega_{21}\omega_{32} + 12\omega_{30}\omega_{32} \\
& + 64\omega_{33} - 256\omega\omega_{33} - 12\omega_{20}\omega_{33} - 192\omega_{20}\omega_{40} - 9\omega_{22}\omega_{40} + 6\omega_{31}\omega_{40} \\
& + 18\omega_{21}\omega_{41} - 6\omega_{30}\omega_{41} - 4\omega_{10} (1524\omega_{21} - 640\omega_{30} - 18\omega_{32} + 9\omega_{41}) \\
& + \omega_{11} (1024 - 4096\omega + 6096\omega_{20} - 216\omega_{22} + 24\omega_{33} + 36\omega_{40} - 18\omega_{42}) \\
& - 48\omega_{42} + 192\omega\omega_{42} + 9\omega_{20}\omega_{42}) \\
& + q^{24} (-7168\omega_{10}^2 + 7296\omega_{20}^2 - 840\omega_{21}^2 - 576\omega_{22} - 7296\omega\omega_{22} + 2200\omega_{21}\omega_{30} \\
& - 640\omega_{30}^2 + 384\omega_{31} + 4864\omega\omega_{31} - 1920\omega_{20}\omega_{31} + 84\omega_{22}\omega_{31} - 56\omega_{31}^2 - 84\omega_{21}\omega_{32} \\
& + 28\omega_{30}\omega_{32} - 192\omega_{33} + 640\omega\omega_{33} - 28\omega_{20}\omega_{33} + 480\omega_{20}\omega_{40} - 21\omega_{22}\omega_{40} \\
& + 14\omega_{31}\omega_{40} + 42\omega_{21}\omega_{41} - 14\omega_{30}\omega_{41} + 4\omega_{10} (3932\omega_{21} - 1216\omega_{30} - 70\omega_{32} + 35\omega_{41}) \\
& + 2\omega_{11} (768 + 3584\omega - 7864\omega_{20} + 420\omega_{22} + 28\omega_{33} - 70\omega_{40} - 21\omega_{42}) \\
& + 144\omega_{42} - 480\omega\omega_{42} + 21\omega_{20}\omega_{42})
\end{aligned}$$

$$\begin{aligned}
& + q^{16} (456704\omega_{10}^2 + 151552\omega_{11} - 142848\omega_{20} + 77136\omega_{11}\omega_{20} - 81408\omega_{20}^2 + 16920\omega_{21}^2 \\
& - 69504\omega_{22} - 16920\omega_{11}\omega_{22} - 21000\omega_{21}\omega_{30} + 5120\omega_{30}^2 + 69376\omega_{31} + 15360\omega_{20}\omega_{31} \\
& + 900\omega_{22}\omega_{31} - 600\omega_{31}^2 - 900\omega_{21}\omega_{32} + 300\omega_{30}\omega_{32} + 3712\omega_{33} + 600\omega_{11}\omega_{33} \\
& - 300\omega_{20}\omega_{33} - 5760\omega_{40} + 2820\omega_{11}\omega_{40} - 3840\omega_{20}\omega_{40} - 225\omega_{22}\omega_{40} + 150\omega_{31}\omega_{40} \\
& + \omega_{10} (-77136\omega_{21} + 54272\omega_{30} + 5640\omega_{32} - 2820\omega_{41}) \\
& - 256\omega (2880 + 1784\omega_{11} - 318\omega_{22} + 212\omega_{31} + 20\omega_{33} - 15\omega_{42}) \\
& + 450\omega_{21}\omega_{41} - 150\omega_{30}\omega_{41} - 2784\omega_{42} - 450\omega_{11}\omega_{42} + 225\omega_{20}\omega_{42}) \\
& + q^{10} (51200\omega_{10}^2 + 25600\omega_{11} - 9216\omega_{20} + 233488\omega_{11}\omega_{20} - 155136\omega_{20}^2 + 15288\omega_{21}^2 \\
& + 14016\omega_{22} - 15288\omega_{11}\omega_{22} - 11240\omega_{21}\omega_{30} + 2048\omega_{30}^2 - 18560\omega_{31} + 6144\omega_{20}\omega_{31} \\
& + 1236\omega_{22}\omega_{31} - 824\omega_{31}^2 - 1236\omega_{21}\omega_{32} + 412\omega_{30}\omega_{32} - 1856\omega_{33} + 824\omega_{11}\omega_{33} \\
& - 412\omega_{20}\omega_{33} + 2304\omega_{40} + 2548\omega_{11}\omega_{40} - 1536\omega_{20}\omega_{40} - 309\omega_{22}\omega_{40} + 206\omega_{31}\omega_{40} \\
& + 618\omega_{21}\omega_{41} - 206\omega_{30}\omega_{41} - 4\omega_{10} (58372\omega_{21} - 25856\omega_{30} + 637(-2\omega_{32} + \omega_{41})) \\
& - 512\omega (864 + 100\omega_{11} - 303\omega_{22} + 202\omega_{31} + 4\omega_{33} - 3\omega_{42}) \\
& + 1392\omega_{42} - 618\omega_{11}\omega_{42} + 309\omega_{20}\omega_{42}) \\
& - 8q^{22} (2176\omega_{10}^2 - 1968\omega_{20}^2 - 228\omega_{21}^2 + 120\omega_{22} + 1968\omega\omega_{22} - 260\omega_{21}\omega_{30} \\
& + 112\omega_{30}^2 - 80\omega_{31} - 1312\omega\omega_{31} + 336\omega_{20}\omega_{31} + 12\omega_{22}\omega_{31} - 8\omega_{31}^2 - 12\omega_{21}\omega_{32} \\
& + 4\omega_{30}\omega_{32} - 8\omega_{33} - 112\omega\omega_{33} - 4\omega_{20}\omega_{33} - 84\omega_{20}\omega_{40} - 3\omega_{22}\omega_{40} \\
& + 2\omega_{31}\omega_{40} + 6\omega_{21}\omega_{41} - 2\omega_{30}\omega_{41} + \omega_{10} (-4168\omega_{21} + 1312\omega_{30} - 76\omega_{32} + 38\omega_{41}) \\
& + 6\omega_{42} + 84\omega\omega_{42} + 3\omega_{20}\omega_{42} - 2\omega_{11} (64 + 1088\omega - 2084\omega_{20} - 114\omega_{22} - 4\omega_{33} + 19\omega_{40} + 3\omega_{42})) \\
& + q^{26} (-4096\omega_{10}^2 + 3840\omega_{20}^2 - 216\omega_{21}^2 - 960\omega_{22} - 3840\omega\omega_{22} + 840\omega_{21}\omega_{30} \\
& - 256\omega_{30}^2 + 640\omega_{31} + 2560\omega\omega_{31} - 768\omega_{20}\omega_{31} - 36\omega_{22}\omega_{31} + 24\omega_{31}^2 + 36\omega_{21}\omega_{32} \\
& - 12\omega_{30}\omega_{32} + 64\omega_{33} + 256\omega\omega_{33} + 12\omega_{20}\omega_{33} + 192\omega_{20}\omega_{40} + 9\omega_{22}\omega_{40} \\
& - 6\omega_{31}\omega_{40} - 18\omega_{21}\omega_{41} + 6\omega_{30}\omega_{41} + 4\omega_{10} (1524\omega_{21} - 640\omega_{30} - 18\omega_{32} + 9\omega_{41}) \\
& - 48\omega_{42} - 192\omega\omega_{42} - 9\omega_{20}\omega_{42} + 2\omega_{11} (512 + 2048\omega - 3048\omega_{20} + 108\omega_{22} - 12\omega_{33} - 18\omega_{40} + 9\omega_{42})) \\
& + q^{20} (-74752\omega_{10}^2 + 109056\omega_{11} - 53760\omega_{20} - 118704\omega_{11}\omega_{20} + 48768\omega_{20}^2 + 3672\omega_{21}^2 \\
& + 8640\omega_{22} - 3672\omega_{11}\omega_{22} - 8520\omega_{21}\omega_{30} + 2432\omega_{30}^2 - 4224\omega_{31} + 7296\omega_{20}\omega_{31} \\
& + 612\omega_{22}\omega_{31} - 408\omega_{31}^2 - 612\omega_{21}\omega_{32} + 204\omega_{30}\omega_{32} + 576\omega_{33} + 408\omega_{11}\omega_{33} \\
& - 204\omega_{20}\omega_{33} - 384\omega_{40} + 612\omega_{11}\omega_{40} - 1824\omega_{20}\omega_{40} - 153\omega_{22}\omega_{40} + 102\omega_{31}\omega_{40} \\
& + 4\omega_{10} (29676\omega_{21} - 8128\omega_{30} + 306\omega_{32} - 153\omega_{41}) \\
& + 306\omega_{21}\omega_{41} - 102\omega_{30}\omega_{41} - 432\omega_{42} - 306\omega_{11}\omega_{42} + 153\omega_{20}\omega_{42} \\
& + 32\omega (-13824 + 2336\omega_{11} - 1524\omega_{22} + 1016\omega_{31} - 76\omega_{33} + 57\omega_{42}))
\end{aligned}$$

$$\begin{aligned}
& -q^8 (-74752\omega_{10}^2 - 109056\omega_{11} + 53760\omega_{20} - 118704\omega_{11}\omega_{20} + 48768\omega_{20}^2 + 3672\omega_{21}^2 \\
& - 8640\omega_{22} - 3672\omega_{11}\omega_{22} - 8520\omega_{21}\omega_{30} + 2432\omega_{30}^2 + 4224\omega_{31} + 7296\omega_{20}\omega_{31} \\
& + 612\omega_{22}\omega_{31} - 408\omega_{31}^2 - 612\omega_{21}\omega_{32} + 204\omega_{30}\omega_{32} - 576\omega_{33} + 408\omega_{11}\omega_{33} \\
& - 204\omega_{20}\omega_{33} + 384\omega_{40} + 612\omega_{11}\omega_{40} - 1824\omega_{20}\omega_{40} - 153\omega_{22}\omega_{40} + 102\omega_{31}\omega_{40} \\
& + 4\omega_{10} (29676\omega_{21} - 8128\omega_{30} + 306\omega_{32} - 153\omega_{41}) \\
& + 306\omega_{21}\omega_{41} - 102\omega_{30}\omega_{41} + 432\omega_{42} - 306\omega_{11}\omega_{42} + 153\omega_{20}\omega_{42} \\
& + 32\omega (13824 + 2336\omega_{11} - 1524\omega_{22} + 1016\omega_{31} - 76\omega_{33} + 57\omega_{42})) \} \\
& - 4\eta q^2 (-1 - q^2 - q^4 + q^8 + q^{10} + q^{12}) \\
& \{ -256\omega_{20}\omega'_{10} - 288\omega_{22}\omega'_{10} - 64\omega_{31}\omega'_{10} - 32\omega_{33}\omega'_{10} + 64\omega_{40}\omega'_{10} + 24\omega_{42}\omega'_{10} \\
& + 256\omega_{10}\omega'_{20} + 288\omega_{21}\omega'_{20} - 64\omega_{30}\omega'_{20} - 48\omega_{32}\omega'_{20} + 24\omega_{41}\omega'_{20} + 64\omega'_{21} \\
& - 256\omega\omega'_{21} - 288\omega_{20}\omega'_{21} + 48\omega_{31}\omega'_{21} + 12\omega_{33}\omega'_{21} - 12\omega_{40}\omega'_{21} - 9\omega_{42}\omega'_{21} \\
& + 64\omega_{11}\omega'_{30} + 64\omega_{20}\omega'_{30} + 48\omega_{22}\omega'_{30} + 32\omega_{31}\omega'_{30} - 16\omega_{40}\omega'_{30} - 64\omega_{10}\omega'_{31} \\
& - 48\omega_{21}\omega'_{31} - 32\omega_{30}\omega'_{31} - 12\omega_{32}\omega'_{31} + 6\omega_{41}\omega'_{31} + 16\omega'_{32} - 64\omega\omega'_{32} \\
& + 48\omega_{11}\omega'_{32} - 48\omega_{20}\omega'_{32} + 12\omega_{31}\omega'_{32} - 3\omega_{40}\omega'_{32} - 64\omega_{10}\omega'_{40} - 48\omega_{21}\omega'_{40} \\
& + 16\omega_{30}\omega'_{40} - 16\omega'_{41} + 64\omega\omega'_{41} + 36\omega_{20}\omega'_{41} + 9\omega_{22}\omega'_{41} - 6\omega_{31}\omega'_{41} \\
& + 12\omega_{10}\omega'_{42} - 9\omega_{21}\omega'_{42} + 3\omega_{30}\omega'_{42} + 4\omega'_{43} - 16\omega\omega'_{43} + 6\omega_{11}\omega'_{43} - 3\omega_{20}\omega'_{43} \\
& - 24q^8 (12288\omega'_{10} + 1840\omega'_{21} + 156\omega'_{32} + 20\omega'_{41} + 15\omega'_{43}) \\
& - 2q^2 (1216\omega_{31}\omega'_{10} + 224\omega_{33}\omega'_{10} + 64\omega_{40}\omega'_{10} - 168\omega_{42}\omega'_{10} \\
& - 4352\omega_{10}\omega'_{20} + 2208\omega_{21}\omega'_{20} - 1024\omega_{30}\omega'_{20} - 144\omega_{32}\omega'_{20} + 72\omega_{41}\omega'_{20} \\
& - 960\omega'_{21} + 4352\omega\omega'_{21} + 144\omega_{31}\omega'_{21} + 12\omega_{33}\omega'_{21} - 36\omega_{40}\omega'_{21} - 9\omega_{42}\omega'_{21} \\
& - 1216\omega_{11}\omega'_{30} - 224\omega_{31}\omega'_{30} + 32\omega_{40}\omega'_{30} + 1216\omega_{10}\omega'_{31} - 144\omega_{21}\omega'_{31} \\
& + 224\omega_{30}\omega'_{31} - 12\omega_{32}\omega'_{31} + 6\omega_{41}\omega'_{31} + 288\omega'_{32} - 1024\omega\omega'_{32} \\
& + 144\omega_{11}\omega'_{32} + 12\omega_{31}\omega'_{32} - 3\omega_{40}\omega'_{32} - 64\omega_{10}\omega'_{40} + 96\omega_{21}\omega'_{40} \\
& - 32\omega_{30}\omega'_{40} - 48\omega'_{41} + 64\omega\omega'_{41} - 6\omega_{31}\omega'_{41} \\
& + \omega_{22} (-2208\omega'_{10} + 144\omega'_{30} + 9\omega'_{41}) + 36\omega_{10}\omega'_{42} - 9\omega_{21}\omega'_{42} + 3\omega_{30}\omega'_{42} \\
& + \omega_{20} (4352\omega'_{10} - 2208\omega'_{21} + 1024\omega'_{30} - 144\omega'_{32} - 132\omega'_{41} - 3\omega'_{43}) \\
& + 32\omega\omega'_{43} + 6\omega_{11}\omega'_{43}) \\
& + 2q^{14} (1216\omega_{31}\omega'_{10} + 224\omega_{33}\omega'_{10} + 64\omega_{40}\omega'_{10} - 168\omega_{42}\omega'_{10} \\
& - 4352\omega_{10}\omega'_{20} + 2208\omega_{21}\omega'_{20} - 1024\omega_{30}\omega'_{20} - 144\omega_{32}\omega'_{20} + 72\omega_{41}\omega'_{20} \\
& + 960\omega'_{21} + 4352\omega\omega'_{21} + 144\omega_{31}\omega'_{21} + 12\omega_{33}\omega'_{21} - 36\omega_{40}\omega'_{21} \\
& - 9\omega_{42}\omega'_{21} - 1216\omega_{11}\omega'_{30} - 224\omega_{31}\omega'_{30} + 32\omega_{40}\omega'_{30} + 1216\omega_{10}\omega'_{31} \\
& - 144\omega_{21}\omega'_{31} + 224\omega_{30}\omega'_{31} - 12\omega_{32}\omega'_{31} + 6\omega_{41}\omega'_{31} - 288\omega'_{32} \\
& - 1024\omega\omega'_{32} + 144\omega_{11}\omega'_{32} + 12\omega_{31}\omega'_{32} - 3\omega_{40}\omega'_{32} - 64\omega_{10}\omega'_{40} \\
& + 96\omega_{21}\omega'_{40} - 32\omega_{30}\omega'_{40} + 48\omega'_{41} + 64\omega\omega'_{41} - 6\omega_{31}\omega'_{41} \\
& + \omega_{22} (-2208\omega'_{10} + 144\omega'_{30} + 9\omega'_{41}) + 36\omega_{10}\omega'_{42} - 9\omega_{21}\omega'_{42} + 3\omega_{30}\omega'_{42} \\
& + \omega_{20} (4352\omega'_{10} - 2208\omega'_{21} + 1024\omega'_{30} - 144\omega'_{32} - 132\omega'_{41} - 3\omega'_{43}) \\
& + 32\omega\omega'_{43} + 6\omega_{11}\omega'_{43})
\end{aligned}$$

$$\begin{aligned}
& -2q^{10} (-4288\omega_{31}\omega'_{10} + 544\omega_{33}\omega'_{10} + 192\omega_{40}\omega'_{10} - 408\omega_{42}\omega'_{10} \\
& - 9984\omega_{10}\omega'_{20} - 5280\omega_{21}\omega'_{20} + 3456\omega_{30}\omega'_{20} + 336\omega_{32}\omega'_{20} - 168\omega_{41}\omega'_{20} \\
& - 7232\omega'_{21} + 9984\omega\omega'_{21} - 336\omega_{31}\omega'_{21} + 36\omega_{33}\omega'_{21} + 84\omega_{40}\omega'_{21} - 27\omega_{42}\omega'_{21} \\
& + 4288\omega_{11}\omega'_{30} - 544\omega_{31}\omega'_{30} + 192\omega_{40}\omega'_{30} - 4288\omega_{10}\omega'_{31} + 336\omega_{21}\omega'_{31} \\
& + 544\omega_{30}\omega'_{31} - 36\omega_{32}\omega'_{31} + 18\omega_{41}\omega'_{31} - 800\omega'_{32} + 3456\omega\omega'_{32} \\
& - 336\omega_{11}\omega'_{32} + 36\omega_{31}\omega'_{32} - 9\omega_{40}\omega'_{32} - 192\omega_{10}\omega'_{40} + 576\omega_{21}\omega'_{40} \\
& - 192\omega_{30}\omega'_{40} - 208\omega'_{41} + 192\omega\omega'_{41} - 18\omega_{31}\omega'_{41} \\
& + 3\omega_{22} (1760\omega'_{10} - 112\omega'_{30} + 9\omega'_{41}) - 84\omega_{10}\omega'_{42} - 27\omega_{21}\omega'_{42} + 9\omega_{30}\omega'_{42} \\
& + \omega_{20} (9984\omega'_{10} + 5280\omega'_{21} - 3456\omega'_{30} + 336\omega'_{32} - 492\omega'_{41} - 9\omega'_{43}) \\
& - 128\omega'_{43} + 192\omega\omega'_{43} + 18\omega_{11}\omega'_{43}) \\
& + 2q^6 (-4288\omega_{31}\omega'_{10} + 544\omega_{33}\omega'_{10} + 192\omega_{40}\omega'_{10} - 408\omega_{42}\omega'_{10} \\
& - 9984\omega_{10}\omega'_{20} - 5280\omega_{21}\omega'_{20} + 3456\omega_{30}\omega'_{20} + 336\omega_{32}\omega'_{20} - 168\omega_{41}\omega'_{20} \\
& + 7232\omega'_{21} + 9984\omega\omega'_{21} - 336\omega_{31}\omega'_{21} + 36\omega_{33}\omega'_{21} + 84\omega_{40}\omega'_{21} - 27\omega_{42}\omega'_{21} \\
& + 4288\omega_{11}\omega'_{30} - 544\omega_{31}\omega'_{30} + 192\omega_{40}\omega'_{30} - 4288\omega_{10}\omega'_{31} + 336\omega_{21}\omega'_{31} \\
& + 544\omega_{30}\omega'_{31} - 36\omega_{32}\omega'_{31} + 18\omega_{41}\omega'_{31} + 800\omega'_{32} + 3456\omega\omega'_{32} \\
& - 336\omega_{11}\omega'_{32} + 36\omega_{31}\omega'_{32} - 9\omega_{40}\omega'_{32} - 192\omega_{10}\omega'_{40} + 576\omega_{21}\omega'_{40} \\
& - 192\omega_{30}\omega'_{40} + 208\omega'_{41} + 192\omega\omega'_{41} - 18\omega_{31}\omega'_{41} \\
& + 3\omega_{22} (1760\omega'_{10} - 112\omega'_{30} + 9\omega'_{41}) - 84\omega_{10}\omega'_{42} - 27\omega_{21}\omega'_{42} + 9\omega_{30}\omega'_{42} \\
& + \omega_{20} (9984\omega'_{10} + 5280\omega'_{21} - 3456\omega'_{30} + 336\omega'_{32} - 492\omega'_{41} - 9\omega'_{43}) \\
& + 128\omega'_{43} + 192\omega\omega'_{43} + 18\omega_{11}\omega'_{43}) \\
& + q^{16} (64\omega_{31}\omega'_{10} + 32\omega_{33}\omega'_{10} - 64\omega_{40}\omega'_{10} - 24\omega_{42}\omega'_{10} \\
& - 256\omega_{10}\omega'_{20} - 288\omega_{21}\omega'_{20} + 64\omega_{30}\omega'_{20} + 48\omega_{32}\omega'_{20} - 24\omega_{41}\omega'_{20} \\
& + 64\omega'_{21} + 256\omega\omega'_{21} - 48\omega_{31}\omega'_{21} - 12\omega_{33}\omega'_{21} + 12\omega_{40}\omega'_{21} + 9\omega_{42}\omega'_{21} \\
& - 64\omega_{11}\omega'_{30} - 32\omega_{31}\omega'_{30} + 16\omega_{40}\omega'_{30} + 64\omega_{10}\omega'_{31} + 48\omega_{21}\omega'_{31} \\
& + 32\omega_{30}\omega'_{31} + 12\omega_{32}\omega'_{31} - 6\omega_{41}\omega'_{31} + 16\omega'_{32} + 64\omega\omega'_{32} - 48\omega_{11}\omega'_{32} \\
& - 12\omega_{31}\omega'_{32} + 3\omega_{40}\omega'_{32} + 64\omega_{10}\omega'_{40} + 48\omega_{21}\omega'_{40} - 16\omega_{30}\omega'_{40} \\
& + 3\omega_{22} (96\omega'_{10} - 16\omega'_{30} - 3\omega'_{41}) - 16\omega'_{41} - 64\omega\omega'_{41} + 6\omega_{31}\omega'_{41} \\
& - 12\omega_{10}\omega'_{42} + 9\omega_{21}\omega'_{42} - 3\omega_{30}\omega'_{42} + 4\omega'_{43} + 16\omega\omega'_{43} \\
& - 6\omega_{11}\omega'_{43} + \omega_{20} (256\omega'_{10} + 288\omega'_{21} - 64\omega'_{30} + 48\omega'_{32} - 36\omega'_{41} + 3\omega'_{43}))
\end{aligned}$$

$$\begin{aligned}
& + 2q^4 (-2880\omega_{31}\omega'_{10} + 96\omega_{33}\omega'_{10} - 64\omega_{40}\omega'_{10} - 72\omega_{42}\omega'_{10} \\
& - 1792\omega_{10}\omega'_{20} - 4704\omega_{21}\omega'_{20} + 256\omega_{30}\omega'_{20} - 336\omega_{32}\omega'_{20} + 168\omega_{41}\omega'_{20} \\
& + 2816\omega'_{21} + 1792\omega\omega'_{21} + 336\omega_{31}\omega'_{21} - 12\omega_{33}\omega'_{21} - 84\omega_{40}\omega'_{21} + 9\omega_{42}\omega'_{21} \\
& + 2880\omega_{11}\omega'_{30} - 96\omega_{31}\omega'_{30} - 32\omega_{40}\omega'_{30} - 2880\omega_{10}\omega'_{31} - 336\omega_{21}\omega'_{31} \\
& + 96\omega_{30}\omega'_{31} + 12\omega_{32}\omega'_{31} - 6\omega_{41}\omega'_{31} + 416\omega'_{32} + 256\omega\omega'_{32} \\
& + 336\omega_{11}\omega'_{32} - 12\omega_{31}\omega'_{32} + 3\omega_{40}\omega'_{32} + 64\omega_{10}\omega'_{40} - 96\omega_{21}\omega'_{40} + 32\omega_{30}\omega'_{40} \\
& + \omega_{22} (4704\omega'_{10} + 336\omega'_{30} - 9\omega'_{41}) - 128\omega'_{41} - 64\omega\omega'_{41} + 6\omega_{31}\omega'_{41} \\
& + 84\omega_{10}\omega'_{42} + 9\omega_{21}\omega'_{42} - 3\omega_{30}\omega'_{42} - 40\omega'_{43} - 32\omega\omega'_{43} - 6\omega_{11}\omega'_{43} \\
& + \omega_{20} (1792\omega'_{10} + 4704\omega'_{21} - 256\omega'_{30} - 336\omega'_{32} + 12\omega'_{41} + 3\omega'_{43})) \\
& - 2q^{12} (-2880\omega_{31}\omega'_{10} + 96\omega_{33}\omega'_{10} - 64\omega_{40}\omega'_{10} - 72\omega_{42}\omega'_{10} \\
& - 1792\omega_{10}\omega'_{20} - 4704\omega_{21}\omega'_{20} + 256\omega_{30}\omega'_{20} - 336\omega_{32}\omega'_{20} + 168\omega_{41}\omega'_{20} \\
& - 2816\omega'_{21} + 1792\omega\omega'_{21} + 336\omega_{31}\omega'_{21} - 12\omega_{33}\omega'_{21} - 84\omega_{40}\omega'_{21} + 9\omega_{42}\omega'_{21} \\
& + 2880\omega_{11}\omega'_{30} - 96\omega_{31}\omega'_{30} - 32\omega_{40}\omega'_{30} - 2880\omega_{10}\omega'_{31} - 336\omega_{21}\omega'_{31} \\
& + 96\omega_{30}\omega'_{31} + 12\omega_{32}\omega'_{31} - 6\omega_{41}\omega'_{31} - 416\omega'_{32} + 256\omega\omega'_{32} \\
& + 336\omega_{11}\omega'_{32} - 12\omega_{31}\omega'_{32} + 3\omega_{40}\omega'_{32} + 64\omega_{10}\omega'_{40} - 96\omega_{21}\omega'_{40} + 32\omega_{30}\omega'_{40} \\
& + \omega_{22} (4704\omega'_{10} + 336\omega'_{30} - 9\omega'_{41}) + 128\omega'_{41} - 64\omega\omega'_{41} + 6\omega_{31}\omega'_{41} \\
& + 84\omega_{10}\omega'_{42} + 9\omega_{21}\omega'_{42} - 3\omega_{30}\omega'_{42} + 40\omega'_{43} - 32\omega\omega'_{43} \\
& - 6\omega_{11}\omega'_{43} + \omega_{20} (1792\omega'_{10} + 4704\omega'_{21} - 256\omega'_{30} - 336\omega'_{32} + 12\omega'_{41} + 3\omega'_{43})) \} \\
& + (-1 + q^4)^3 (1 + q^2 + 2q^4 + q^6 + q^8) \\
& (\omega'_{32}\omega'_{41} - \omega'_{31}\omega'_{42} + \omega'_{21}\omega'_{43} \\
& + q^4 (-7040\omega'_{20}\omega'_{31} + 7040\omega'_{10}\omega'_{32} - 160\omega'_{31}\omega'_{40} + 160\omega'_{30}\omega'_{41} - 33\omega'_{32}\omega'_{41} \\
& + 33\omega'_{31}\omega'_{42} + 11\omega'_{21} (640\omega'_{30} - 3\omega'_{43}) - 160\omega'_{10}\omega'_{43}) \\
& + q^8 (-7040\omega'_{20}\omega'_{31} + 7040\omega'_{10}\omega'_{32} - 160\omega'_{31}\omega'_{40} + 160\omega'_{30}\omega'_{41} - 33\omega'_{32}\omega'_{41} \\
& + 33\omega'_{31}\omega'_{42} + 11\omega'_{21} (640\omega'_{30} - 3\omega'_{43}) - 160\omega'_{10}\omega'_{43}) \\
& + q^{12} (\omega'_{32}\omega'_{41} - \omega'_{31}\omega'_{42} + \omega'_{21}\omega'_{43}) \\
& + q^2 (320\omega'_{20}\omega'_{31} - 320\omega'_{10}\omega'_{32} - 80\omega'_{31}\omega'_{40} + 80\omega'_{30}\omega'_{41} + 6\omega'_{32}\omega'_{41} - 6\omega'_{31}\omega'_{42} \\
& - 80\omega'_{10}\omega'_{43} + \omega'_{21} (-320\omega'_{30} + 6\omega'_{43})) \\
& + q^{10} (320\omega'_{20}\omega'_{31} - 320\omega'_{10}\omega'_{32} - 80\omega'_{31}\omega'_{40} + 80\omega'_{30}\omega'_{41} + 6\omega'_{32}\omega'_{41} - 6\omega'_{31}\omega'_{42} \\
& - 80\omega'_{10}\omega'_{43} + \omega'_{21} (-320\omega'_{30} + 6\omega'_{43})) \\
& + 4q^6 (-96\omega'_{20}\omega'_{31} + 96\omega'_{10}\omega'_{32} + 120\omega'_{31}\omega'_{40} - 120\omega'_{30}\omega'_{41} + 13\omega'_{32}\omega'_{41} \\
& - 13\omega'_{31}\omega'_{42} + 120\omega'_{10}\omega'_{43} + \omega'_{21} (96\omega'_{30} + 13\omega'_{43})) \} \\
& / (1179648\eta^2 q^{10} (-1 - q^2 - q^4 + q^8 + q^{10} + q^{12}))
\end{aligned}$$

$$\begin{aligned}
\langle \sigma_1^x \sigma_5^x \rangle = & \\
& \{-8\eta^2 q^2 \{ 512\omega_{10}^2 + 128\omega_{11} - 512\omega\omega_{11} + 272\omega_{11}\omega_{20} - 192\omega_{20}^2 - 272\omega_{10}\omega_{21} \\
& - 168\omega_{21}^2 - 48\omega_{22} + 192\omega\omega_{22} + 168\omega_{11}\omega_{22} + 128\omega_{10}\omega_{30} + 248\omega_{21}\omega_{30} \\
& - 64\omega_{30}^2 + 32\omega_{31} - 128\omega\omega_{31} - 192\omega_{20}\omega_{31} - 12\omega_{22}\omega_{31} + 8\omega_{31}^2 \\
& - 56\omega_{10}\omega_{32} + 12\omega_{21}\omega_{32} - 4\omega_{30}\omega_{32} - 16\omega_{33} + 64\omega\omega_{33} - 8\omega_{11}\omega_{33} \\
& + 4\omega_{20}\omega_{33} - 28\omega_{11}\omega_{40} + 48\omega_{20}\omega_{40} + 3\omega_{22}\omega_{40} - 2\omega_{31}\omega_{40} + 28\omega_{10}\omega_{41} \\
& - 6\omega_{21}\omega_{41} + 2\omega_{30}\omega_{41} + 12\omega_{42} - 48\omega\omega_{42} + 6\omega_{11}\omega_{42} - 3\omega_{20}\omega_{42} \\
& + q^{14} (-306688\omega_{10}^2 - 159872\omega_{11} + 133632\omega_{20} - 266928\omega_{11}\omega_{20} + 170304\omega_{20}^2 \\
& - 26568\omega_{21}^2 + 31152\omega_{22} + 26568\omega_{11}\omega_{22} + 18264\omega_{21}\omega_{30} - 3136\omega_{30}^2 - 25376\omega_{31} \\
& - 9408\omega_{20}\omega_{31} - 2268\omega_{22}\omega_{31} + 1512\omega_{31}^2 + 2268\omega_{21}\omega_{32} - 756\omega_{30}\omega_{32} - 368\omega_{33} \\
& - 1512\omega_{11}\omega_{33} + 756\omega_{20}\omega_{33} + 1152\omega_{40} - 4428\omega_{11}\omega_{40} + 2352\omega_{20}\omega_{40} \\
& + 567\omega_{22}\omega_{40} - 378\omega_{31}\omega_{40} - 1134\omega_{21}\omega_{41} + 378\omega_{30}\omega_{41} \\
& + 4\omega_{10}(66732\omega_{21} - 28384\omega_{30} + 1107(-2\omega_{32} + \omega_{41})) \\
& + 16\omega(129024 + 19168\omega_{11} - 10644\omega_{22} + 7096\omega_{31} + 196\omega_{33} - 147\omega_{42}) \\
& + 276\omega_{42} + 1134\omega_{11}\omega_{42} - 567\omega_{20}\omega_{42}) \\
& + q^{10}(218112\omega_{10}^2 + 166144\omega_{11} - 110592\omega_{20} - 180432\omega_{11}\omega_{20} + 79488\omega_{20}^2 \\
& - 2808\omega_{21}^2 - 9888\omega_{22} + 2808\omega_{11}\omega_{22} - 4824\omega_{21}\omega_{30} + 1920\omega_{30}^2 + 6592\omega_{31} \\
& + 5760\omega_{20}\omega_{31} - 972\omega_{22}\omega_{31} + 648\omega_{31}^2 + 972\omega_{21}\omega_{32} - 324\omega_{30}\omega_{32} - 224\omega_{33} \\
& - 648\omega_{11}\omega_{33} + 324\omega_{20}\omega_{33} - 468\omega_{11}\omega_{40} - 1440\omega_{20}\omega_{40} + 243\omega_{22}\omega_{40} \\
& - 486\omega_{21}\omega_{41} + 162\omega_{30}\omega_{41} + 36\omega_{10}(5012\omega_{21} - 1472\omega_{30} - 26\omega_{32} + 13\omega_{41}) \\
& - 96\omega(-3072 + 2272\omega_{11} + 828\omega_{22} - 552\omega_{31} + 20\omega_{33} - 15\omega_{42}) \\
& - 162\omega_{31}\omega_{40} + 168\omega_{42} + 486\omega_{11}\omega_{42} - 243\omega_{20}\omega_{42}) \\
& + q^{26}(80896\omega_{10}^2 + 27648\omega_{20} - 21120\omega_{20}^2 - 360\omega_{21}^2 + 2400\omega_{22} + 21120\omega\omega_{22} \\
& - 1800\omega_{21}\omega_{30} + 640\omega_{30}^2 - 1600\omega_{31} - 14080\omega\omega_{31} + 1920\omega_{20}\omega_{31} - 324\omega_{22}\omega_{31} \\
& + 216\omega_{31}^2 + 324\omega_{21}\omega_{32} - 108\omega_{30}\omega_{32} + 32\omega_{33} - 640\omega\omega_{33} + 108\omega_{20}\omega_{33} \\
& - 480\omega_{20}\omega_{40} + 81\omega_{22}\omega_{40} - 54\omega_{31}\omega_{40} - 162\omega_{21}\omega_{41} + 54\omega_{30}\omega_{41} \\
& - 4\omega_{10}(10596\omega_{21} - 5(704\omega_{30} - 6\omega_{32} + 3\omega_{41})) \\
& - 2\omega_{11}(22400 + 40448\omega - 21192\omega_{20} - 180\omega_{22} + 108\omega_{33} + 30\omega_{40} - 81\omega_{42}) \\
& - 24\omega_{42} + 480\omega\omega_{42} - 81\omega_{20}\omega_{42})
\end{aligned}$$

$$\begin{aligned}
& + q^{30}(-512\omega_{10}^2 + 192\omega_{20}^2 + 168\omega_{21}^2 - 48\omega_{22} - 192\omega\omega_{22} - 248\omega_{21}\omega_{30} \\
& + 64\omega_{30}^2 + 32\omega_{31} + 128\omega\omega_{31} + 192\omega_{20}\omega_{31} + 12\omega_{22}\omega_{31} - 8\omega_{31}^2 \\
& - 12\omega_{21}\omega_{32} + 4\omega_{30}\omega_{32} - 16\omega_{33} - 64\omega\omega_{33} - 4\omega_{20}\omega_{33} - 48\omega_{20}\omega_{40} \\
& - 3\omega_{22}\omega_{40} + 2\omega_{31}\omega_{40} + 4\omega_{10}(68\omega_{21} - 32\omega_{30} + 14\omega_{32} - 7\omega_{41}) \\
& + 6\omega_{21}\omega_{41} - 2\omega_{30}\omega_{41} + 2\omega_{11}(64 + 256\omega - 136\omega_{20} - 84\omega_{22} \\
& + 4\omega_{33} + 14\omega_{40} - 3\omega_{42}) \\
& + 12\omega_{42} + 48\omega\omega_{42} + 3\omega_{20}\omega_{42}) \\
& + q^4(-80896\omega_{10}^2 + 27648\omega_{20} + 21120\omega_{20}^2 + 360\omega_{21}^2 + 2400\omega_{22} \\
& - 21120\omega\omega_{22} + 1800\omega_{21}\omega_{30} - 640\omega_{30}^2 - 1600\omega_{31} + 14080\omega\omega_{31} \\
& - 1920\omega_{20}\omega_{31} + 324\omega_{22}\omega_{31} - 216\omega_{31}^2 - 324\omega_{21}\omega_{32} + 108\omega_{30}\omega_{32} \\
& + 32\omega_{33} + 640\omega\omega_{33} - 108\omega_{20}\omega_{33} + 480\omega_{20}\omega_{40} - 81\omega_{22}\omega_{40} \\
& + 54\omega_{31}\omega_{40} + 162\omega_{21}\omega_{41} - 54\omega_{30}\omega_{41} \\
& + 4\omega_{10}(10596\omega_{21} - 5(704\omega_{30} - 6\omega_{32} + 3\omega_{41})) \\
& + 2\omega_{11}(-22400 + 40448\omega - 21192\omega_{20} - 180\omega_{22} + 108\omega_{33} + 30\omega_{40} - 81\omega_{42}) \\
& - 24\omega_{42} - 480\omega\omega_{42} + 81\omega_{20}\omega_{42}) \\
& - q^6(89600\omega_{10}^2 - 56064\omega_{20} - 58944\omega_{20}^2 + 4488\omega_{21}^2 + 624\omega_{22} + 58944\omega\omega_{22} \\
& - 7064\omega_{21}\omega_{30} + 1856\omega_{30}^2 - 1184\omega_{31} - 39296\omega\omega_{31} + 5568\omega_{20}\omega_{31} \\
& + 444\omega_{22}\omega_{31} - 296\omega_{31}^2 - 444\omega_{21}\omega_{32} + 148\omega_{30}\omega_{32} - 176\omega_{33} - 1856\omega\omega_{33} \\
& - 148\omega_{20}\omega_{33} + 192\omega_{40} - 1392\omega_{20}\omega_{40} - 111\omega_{22}\omega_{40} + 74\omega_{31}\omega_{40} + 222\omega_{21}\omega_{41} \\
& - 74\omega_{30}\omega_{41} - 4\omega_{10}(26668\omega_{21} - 9824\omega_{30} + 187(-2\omega_{32} + \omega_{41})) \\
& + \omega_{11}(104320 - 89600\omega + 106672\omega_{20} - 4488\omega_{22} + 296\omega_{33} + 748\omega_{40} - 222\omega_{42}) \\
& + 132\omega_{42} + 1392\omega\omega_{42} + 111\omega_{20}\omega_{42}) \\
& + q^{20}(-218112\omega_{10}^2 + 166144\omega_{11} - 110592\omega_{20} + 180432\omega_{11}\omega_{20} - 79488\omega_{20}^2 \\
& + 2808\omega_{21}^2 - 9888\omega_{22} - 2808\omega_{11}\omega_{22} + 4824\omega_{21}\omega_{30} - 1920\omega_{30}^2 + 6592\omega_{31} \\
& - 5760\omega_{20}\omega_{31} + 972\omega_{22}\omega_{31} - 648\omega_{31}^2 - 972\omega_{21}\omega_{32} + 324\omega_{30}\omega_{32} - 224\omega_{33} \\
& + 648\omega_{11}\omega_{33} - 324\omega_{20}\omega_{33} + 468\omega_{11}\omega_{40} + 1440\omega_{20}\omega_{40} - 243\omega_{22}\omega_{40} \\
& + 162\omega_{31}\omega_{40} + 486\omega_{21}\omega_{41} - 162\omega_{30}\omega_{41} \\
& - 36\omega_{10}(5012\omega_{21} - 1472\omega_{30} - 26\omega_{32} + 13\omega_{41}) \\
& + 96\omega(3072 + 2272\omega_{11} + 828\omega_{22} - 552\omega_{31} + 20\omega_{33} - 15\omega_{42}) \\
& + 168\omega_{42} - 486\omega_{11}\omega_{42} + 243\omega_{20}\omega_{42})
\end{aligned}$$

$$\begin{aligned}
& + q^{16}(306688\omega_{10}^2 - 159872\omega_{11} + 133632\omega_{20} + 266928\omega_{11}\omega_{20} - 170304\omega_{20}^2 \\
& + 26568\omega_{21}^2 + 31152\omega_{22} - 26568\omega_{11}\omega_{22} - 18264\omega_{21}\omega_{30} + 3136\omega_{30}^2 - 25376\omega_{31} \\
& + 9408\omega_{20}\omega_{31} + 2268\omega_{22}\omega_{31} - 1512\omega_{31}^2 - 2268\omega_{21}\omega_{32} + 756\omega_{30}\omega_{32} - 368\omega_{33} \\
& + 1512\omega_{11}\omega_{33} - 756\omega_{20}\omega_{33} + 1152\omega_{40} + 4428\omega_{11}\omega_{40} - 2352\omega_{20}\omega_{40} - 567\omega_{22}\omega_{40} \\
& + 378\omega_{31}\omega_{40} + 1134\omega_{21}\omega_{41} - 378\omega_{30}\omega_{41} \\
& - 4\omega_{10}(66732\omega_{21} - 28384\omega_{30} + 1107(-2\omega_{32} + \omega_{41})) \\
& - 16\omega(-129024 + 19168\omega_{11} - 10644\omega_{22} + 7096\omega_{31} + 196\omega_{33} - 147\omega_{42}) \\
& + 276\omega_{42} - 1134\omega_{11}\omega_{42} + 567\omega_{20}\omega_{42}) \\
& + q^2(2048\omega_{10}^2 + 1200\omega_{11}\omega_{20} - 768\omega_{20}^2 + 648\omega_{21}^2 - 648\omega_{11}\omega_{22} + 552\omega_{21}\omega_{30} \\
& - 256\omega_{30}^2 - 768\omega_{20}\omega_{31} - 108\omega_{22}\omega_{31} + 72\omega_{31}^2 + 108\omega_{21}\omega_{32} - 36\omega_{30}\omega_{32} \\
& - 72\omega_{11}\omega_{33} + 36\omega_{20}\omega_{33} + 108\omega_{11}\omega_{40} + 192\omega_{20}\omega_{40} + 27\omega_{22}\omega_{40} - 18\omega_{31}\omega_{40} \\
& - 54\omega_{21}\omega_{41} + 18\omega_{30}\omega_{41} - 4\omega_{10}(300\omega_{21} - 128\omega_{30} - 54\omega_{32} + 27\omega_{41}) \\
& + 54\omega_{11}\omega_{42} - 27\omega_{20}\omega_{42} - 64\omega(32\omega_{11} - 12\omega_{22} + 8\omega_{31} - 4\omega_{33} + 3\omega_{42})) \\
& + q^{28}(-2048\omega_{10}^2 - 1200\omega_{11}\omega_{20} + 768\omega_{20}^2 - 648\omega_{21}^2 + 648\omega_{11}\omega_{22} - 552\omega_{21}\omega_{30} \\
& + 256\omega_{30}^2 + 768\omega_{20}\omega_{31} + 108\omega_{22}\omega_{31} - 72\omega_{31}^2 - 108\omega_{21}\omega_{32} + 36\omega_{30}\omega_{32} \\
& + 72\omega_{11}\omega_{33} - 36\omega_{20}\omega_{33} - 108\omega_{11}\omega_{40} - 192\omega_{20}\omega_{40} - 27\omega_{22}\omega_{40} + 18\omega_{31}\omega_{40} \\
& + 54\omega_{21}\omega_{41} - 18\omega_{30}\omega_{41} + 4\omega_{10}(300\omega_{21} - 128\omega_{30} - 54\omega_{32} + 27\omega_{41}) \\
& - 54\omega_{11}\omega_{42} + 27\omega_{20}\omega_{42} + 64\omega(32\omega_{11} - 12\omega_{22} + 8\omega_{31} - 4\omega_{33} + 3\omega_{42})) \\
& + q^{18}(157696\omega_{10}^2 + 194048\omega_{11} - 132096\omega_{20} + 226960\omega_{11}\omega_{20} - 119040\omega_{20}^2 \\
& - 9768\omega_{21}^2 - 27840\omega_{22} + 9768\omega_{11}\omega_{22} + 16312\omega_{21}\omega_{30} - 4352\omega_{30}^2 + 24704\omega_{31} \\
& - 13056\omega_{20}\omega_{31} - 1284\omega_{22}\omega_{31} + 856\omega_{31}^2 + 1284\omega_{21}\omega_{32} - 428\omega_{30}\omega_{32} + 704\omega_{33} \\
& - 856\omega_{11}\omega_{33} + 428\omega_{20}\omega_{33} - 1536\omega_{40} - 1628\omega_{11}\omega_{40} + 3264\omega_{20}\omega_{40} \\
& + 321\omega_{22}\omega_{40} - 214\omega_{31}\omega_{40} - 4\omega_{10}(56740\omega_{21} - 19840\omega_{30} + 814\omega_{32} - 407\omega_{41}) \\
& - 642\omega_{21}\omega_{41} + 214\omega_{30}\omega_{41} - 528\omega_{42} + 642\omega_{11}\omega_{42} - 321\omega_{20}\omega_{42} \\
& - 64\omega(-18432 + 2464\omega_{11} - 1860\omega_{22} + 1240\omega_{31} - 68\omega_{33} + 51\omega_{42})) \\
& + q^{12}(-157696\omega_{10}^2 + 194048\omega_{11} - 132096\omega_{20} - 226960\omega_{11}\omega_{20} + 119040\omega_{20}^2 \\
& + 9768\omega_{21}^2 - 27840\omega_{22} - 9768\omega_{11}\omega_{22} - 16312\omega_{21}\omega_{30} + 4352\omega_{30}^2 + 24704\omega_{31} \\
& + 13056\omega_{20}\omega_{31} + 1284\omega_{22}\omega_{31} - 856\omega_{31}^2 - 1284\omega_{21}\omega_{32} + 428\omega_{30}\omega_{32} \\
& + 704\omega_{33} + 856\omega_{11}\omega_{33} - 428\omega_{20}\omega_{33} - 1536\omega_{40} + 1628\omega_{11}\omega_{40} - 3264\omega_{20}\omega_{40} \\
& - 321\omega_{22}\omega_{40} + 214\omega_{31}\omega_{40} + 4\omega_{10}(56740\omega_{21} - 19840\omega_{30} + 814\omega_{32} - 407\omega_{41}) \\
& + 642\omega_{21}\omega_{41} - 214\omega_{30}\omega_{41} - 528\omega_{42} - 642\omega_{11}\omega_{42} + 321\omega_{20}\omega_{42} \\
& + 64\omega(18432 + 2464\omega_{11} - 1860\omega_{22} + 1240\omega_{31} - 68\omega_{33} + 51\omega_{42}))
\end{aligned}$$

$$\begin{aligned}
& + q^{24}(89600\omega_{10}^2 + 56064\omega_{20} - 58944\omega_{20}^2 + 4488\omega_{21}^2 - 624\omega_{22} + 58944\omega\omega_{22} \\
& - 7064\omega_{21}\omega_{30} + 1856\omega_{30}^2 + 1184\omega_{31} - 39296\omega\omega_{31} + 5568\omega_{20}\omega_{31} + 444\omega_{22}\omega_{31} \\
& - 296\omega_{31}^2 - 444\omega_{21}\omega_{32} + 148\omega_{30}\omega_{32} + 176\omega_{33} - 1856\omega\omega_{33} - 148\omega_{20}\omega_{33} - 192\omega_{40} \\
& - 1392\omega_{20}\omega_{40} - 111\omega_{22}\omega_{40} + 74\omega_{31}\omega_{40} + 222\omega_{21}\omega_{41} - 74\omega_{30}\omega_{41} \\
& - 4\omega_{10}(26668\omega_{21} - 9824\omega_{30} + 187(-2\omega_{32} + \omega_{41})) \\
& - 132\omega_{42} + 1392\omega\omega_{42} + 111\omega_{20}\omega_{42} - 2\omega_{11}(52160 + 44800\omega - 53336\omega_{20} \\
& + 2244\omega_{22} - 148\omega_{33} - 374\omega_{40} + 111\omega_{42})) \\
& + q^{22}(-193024\omega_{10}^2 + 25344\omega_{20} - 45120\omega_{20}^2 - 5976\omega_{21}^2 + 4848\omega_{22} \\
& + 45120\omega\omega_{22} + 5640\omega_{21}\omega_{30} - 1216\omega_{30}^2 - 5536\omega_{31} - 30080\omega\omega_{31} \\
& - 3648\omega_{20}\omega_{31} - 756\omega_{22}\omega_{31} + 504\omega_{31}^2 + 756\omega_{21}\omega_{32} - 252\omega_{30}\omega_{32} \\
& - 304\omega_{33} + 1216\omega\omega_{33} + 252\omega_{20}\omega_{33} + 576\omega_{40} + 912\omega_{20}\omega_{40} + 189\omega_{22}\omega_{40} \\
& - 126\omega_{31}\omega_{40} - 4\omega_{10}(25884\omega_{21} - 7520\omega_{30} + 498\omega_{32} - 249\omega_{41}) \\
& - 378\omega_{21}\omega_{41} + 126\omega_{30}\omega_{41} + 228\omega_{42} - 912\omega\omega_{42} - 189\omega_{20}\omega_{42} \\
& + 2\omega_{11}(-25664 + 96512\omega + 51768\omega_{20} + 2988\omega_{22} - 252\omega_{33} - 498\omega_{40} + 189\omega_{42})) \\
& + q^8(193024\omega_{10}^2 + 25344\omega_{20} + 45120\omega_{20}^2 + 5976\omega_{21}^2 + 4848\omega_{22} - 45120\omega\omega_{22} \\
& - 5640\omega_{21}\omega_{30} + 1216\omega_{30}^2 - 5536\omega_{31} + 30080\omega\omega_{31} + 3648\omega_{20}\omega_{31} + 756\omega_{22}\omega_{31} \\
& - 504\omega_{31}^2 - 756\omega_{21}\omega_{32} + 252\omega_{30}\omega_{32} - 304\omega_{33} - 1216\omega\omega_{33} - 252\omega_{20}\omega_{33} \\
& + 576\omega_{40} - 912\omega_{20}\omega_{40} - 189\omega_{22}\omega_{40} + 126\omega_{31}\omega_{40} \\
& + 4\omega_{10}(25884\omega_{21} - 7520\omega_{30} + 498\omega_{32} - 249\omega_{41}) \\
& + 378\omega_{21}\omega_{41} - 126\omega_{30}\omega_{41} + 228\omega_{42} + 912\omega\omega_{42} + 189\omega_{20}\omega_{42} \\
& - 2\omega_{11}(25664 + 96512\omega + 51768\omega_{20} + 2988\omega_{22} - 252\omega_{33} - 498\omega_{40} + 189\omega_{42}))\}
\end{aligned}$$

$$\begin{aligned}
& + (-1 + q^2)^3(1 + q^2)^2(1 + q^2 + 2q^4 + q^6 + q^8) \\
& \{ -32(1 - 10q^2 - 256q^4 - 342q^6 - 514q^8 - 342q^{10} - 256q^{12} - 10q^{14} + q^{16})\omega'_{20}\omega'_{31} \\
& + 32\omega'_{10}\omega'_{32} - 320q^2\omega'_{10}\omega'_{32} - 8192q^4\omega'_{10}\omega'_{32} - 10944q^6\omega'_{10}\omega'_{32} - 16448q^8\omega'_{10}\omega'_{32} \\
& - 10944q^{10}\omega'_{10}\omega'_{32} - 8192q^{12}\omega'_{10}\omega'_{32} - 320q^{14}\omega'_{10}\omega'_{32} + 32q^{16}\omega'_{10}\omega'_{32} + 8\omega'_{31}\omega'_{40} \\
& + 112q^2\omega'_{31}\omega'_{40} + 256q^4\omega'_{31}\omega'_{40} - 240q^6\omega'_{31}\omega'_{40} - 272q^8\omega'_{31}\omega'_{40} - 240q^{10}\omega'_{31}\omega'_{40} \\
& + 256q^{12}\omega'_{31}\omega'_{40} + 112q^{14}\omega'_{31}\omega'_{40} + 8q^{16}\omega'_{31}\omega'_{40} - 8\omega'_{30}\omega'_{41} - 112q^2\omega'_{30}\omega'_{41} \\
& - 256q^4\omega'_{30}\omega'_{41} + 240q^6\omega'_{30}\omega'_{41} + 272q^8\omega'_{30}\omega'_{41} + 240q^{10}\omega'_{30}\omega'_{41} - 256q^{12}\omega'_{30}\omega'_{41} \\
& - 112q^{14}\omega'_{30}\omega'_{41} - 8q^{16}\omega'_{30}\omega'_{41} - 3\omega'_{32}\omega'_{41} + 2q^2\omega'_{32}\omega'_{41} + 30q^6\omega'_{32}\omega'_{41} - 58q^8\omega'_{32}\omega'_{41} \\
& + 30q^{10}\omega'_{32}\omega'_{41} + 2q^{14}\omega'_{32}\omega'_{41} - 3q^{16}\omega'_{32}\omega'_{41} + 3\omega'_{31}\omega'_{42} - 2q^2\omega'_{31}\omega'_{42} - 30q^6\omega'_{31}\omega'_{42} \\
& + 58q^8\omega'_{31}\omega'_{42} - 30q^{10}\omega'_{31}\omega'_{42} - 2q^{14}\omega'_{31}\omega'_{42} + 3q^{16}\omega'_{31}\omega'_{42} + 8\omega'_{10}\omega'_{43} + 112q^2\omega'_{10}\omega'_{43} \\
& + 256q^4\omega'_{10}\omega'_{43} - 240q^6\omega'_{10}\omega'_{43} - 272q^8\omega'_{10}\omega'_{43} - 240q^{10}\omega'_{10}\omega'_{43} + 256q^{12}\omega'_{10}\omega'_{43} \\
& + 112q^{14}\omega'_{10}\omega'_{43} + 8q^{16}\omega'_{10}\omega'_{43} + \omega'_{21} (\\
& 32(1 - 10q^2 - 256q^4 - 342q^6 - 514q^8 - 342q^{10} - 256q^{12} - 10q^{14} + q^{16})\omega'_{30} \\
& - (-1 + q^2)^4(3 + 10q^2 + 22q^4 + 10q^6 + 3q^8)\omega'_{43}) \} \\
& - 2\eta(-1 - q^2 - q^4 + q^8 + q^{10} + q^{12}) \\
& \{ -16\omega_{31}\omega'_{21} - 4\omega_{33}\omega'_{21} + 4\omega_{40}\omega'_{21} + 3\omega_{42}\omega'_{21} + 16\omega_{21}\omega'_{31} + 4\omega_{32}\omega'_{31} - 2\omega_{41}\omega'_{31} \\
& - 16\omega_{11}\omega'_{32} - 4\omega_{31}\omega'_{32} + \omega_{40}\omega'_{32} - 4\omega_{20}\omega'_{41} - 3\omega_{22}\omega'_{41} + 2\omega_{31}\omega'_{41} + 4\omega_{10}\omega'_{42} \\
& + 3\omega_{21}\omega'_{42} - \omega_{30}\omega'_{42} - 2\omega_{11}\omega'_{43} + \omega_{20}\omega'_{43} \\
& + q^4(8064\omega_{31}\omega'_{10} + 960\omega_{33}\omega'_{10} - 1024\omega_{40}\omega'_{10} - 720\omega_{42}\omega'_{10} + 11264\omega_{10}\omega'_{20} \\
& + 5952\omega_{21}\omega'_{20} - 3200\omega_{30}\omega'_{20} - 480\omega_{32}\omega'_{20} + 240\omega_{41}\omega'_{20} + 1920\omega'_{21} - 11264\omega\omega'_{21} \\
& + 464\omega_{31}\omega'_{21} - 28\omega_{33}\omega'_{21} - 116\omega_{40}\omega'_{21} + 21\omega_{42}\omega'_{21} - 8064\omega_{11}\omega'_{30} - 960\omega_{31}\omega'_{30} \\
& + 160\omega_{40}\omega'_{30} + 8064\omega_{10}\omega'_{31} - 464\omega_{21}\omega'_{31} + 960\omega_{30}\omega'_{31} + 28\omega_{32}\omega'_{31} - 14\omega_{41}\omega'_{31} \\
& + 768\omega'_{32} - 3200\omega\omega'_{32} + 464\omega_{11}\omega'_{32} - 28\omega_{31}\omega'_{32} + 7\omega_{40}\omega'_{32} + 1024\omega_{10}\omega'_{40} \\
& + 480\omega_{21}\omega'_{40} - 160\omega_{30}\omega'_{40} + 96\omega'_{41} - 1024\omega\omega'_{41} + 14\omega_{31}\omega'_{41} \\
& - 3\omega_{22}(1984\omega'_{10} - 160\omega'_{30} + 7\omega'_{41}) + 124\omega_{10}\omega'_{42} + 21\omega_{21}\omega'_{42} - 7\omega_{30}\omega'_{42} \\
& - \omega_{20}(11264\omega'_{10} + 5952\omega'_{21} - 3200\omega'_{30} + 480\omega'_{32} + 604\omega'_{41} - 7\omega'_{43}) \\
& + 48\omega'_{43} + 160\omega\omega'_{43} - 14\omega_{11}\omega'_{43})
\end{aligned}$$

$$\begin{aligned}
& + q^{20}(-384\omega_{31}\omega'_{10} - 192\omega_{33}\omega'_{10} - 128\omega_{40}\omega'_{10} + 144\omega_{42}\omega'_{10} - 3584\omega_{10}\omega'_{20} \\
& - 1344\omega_{21}\omega'_{20} + 512\omega_{30}\omega'_{20} - 96\omega_{32}\omega'_{20} + 48\omega_{41}\omega'_{20} + 896\omega'_{21} \\
& + 3584\omega\omega'_{21} + 16\omega_{31}\omega'_{21} + 4\omega_{33}\omega'_{21} - 4\omega_{40}\omega'_{21} - 3\omega_{42}\omega'_{21} + 384\omega_{11}\omega'_{30} \\
& + 192\omega_{31}\omega'_{30} - 64\omega_{40}\omega'_{30} - 384\omega_{10}\omega'_{31} - 16\omega_{21}\omega'_{31} - 192\omega_{30}\omega'_{31} - 4\omega_{32}\omega'_{31} \\
& + 2\omega_{41}\omega'_{31} + 128\omega'_{32} + 512\omega\omega'_{32} + 16\omega_{11}\omega'_{32} + 4\omega_{31}\omega'_{32} - \omega_{40}\omega'_{32} + 128\omega_{10}\omega'_{40} \\
& - 192\omega_{21}\omega'_{40} + 64\omega_{30}\omega'_{40} - 32\omega'_{41} - 128\omega\omega'_{41} - 2\omega_{31}\omega'_{41} \\
& + 3\omega_{22}(448\omega'_{10} + 32\omega'_{30} + \omega'_{41}) + 44\omega_{10}\omega'_{42} - 3\omega_{21}\omega'_{42} + \omega_{30}\omega'_{42} \\
& + \omega_{20}(3584\omega'_{10} + 1344\omega'_{21} - 512\omega'_{30} - 96\omega'_{32} + 148\omega'_{41} - \omega'_{43}) \\
& - 16\omega'_{43} - 64\omega\omega'_{43} + 2\omega_{11}\omega'_{43}) \\
& + q^{18}(-8064\omega_{31}\omega'_{10} - 960\omega_{33}\omega'_{10} + 1024\omega_{40}\omega'_{10} + 720\omega_{42}\omega'_{10} - 11264\omega_{10}\omega'_{20} \\
& - 5952\omega_{21}\omega'_{20} + 3200\omega_{30}\omega'_{20} + 480\omega_{32}\omega'_{20} - 240\omega_{41}\omega'_{20} + 1920\omega'_{21} + 11264\omega\omega'_{21} \\
& - 464\omega_{31}\omega'_{21} + 28\omega_{33}\omega'_{21} + 116\omega_{40}\omega'_{21} - 21\omega_{42}\omega'_{21} + 8064\omega_{11}\omega'_{30} + 960\omega_{31}\omega'_{30} \\
& - 160\omega_{40}\omega'_{30} - 8064\omega_{10}\omega'_{31} + 464\omega_{21}\omega'_{31} - 960\omega_{30}\omega'_{31} - 28\omega_{32}\omega'_{31} + 14\omega_{41}\omega'_{31} \\
& + 768\omega'_{32} + 3200\omega\omega'_{32} - 464\omega_{11}\omega'_{32} + 28\omega_{31}\omega'_{32} - 7\omega_{40}\omega'_{32} - 1024\omega_{10}\omega'_{40} \\
& - 480\omega_{21}\omega'_{40} + 160\omega_{30}\omega'_{40} + 96\omega'_{41} + 1024\omega\omega'_{41} - 14\omega_{31}\omega'_{41} \\
& + 3\omega_{22}(1984\omega'_{10} - 160\omega'_{30} + 7\omega'_{41}) - 124\omega_{10}\omega'_{42} - 21\omega_{21}\omega'_{42} + 7\omega_{30}\omega'_{42} \\
& + \omega_{20}(11264\omega'_{10} + 5952\omega'_{21} - 3200\omega'_{30} + 480\omega'_{32} + 604\omega'_{41} - 7\omega'_{43}) \\
& + 48\omega'_{43} - 160\omega\omega'_{43} + 14\omega_{11}\omega'_{43}) \\
& + q^6(32(4608 + 3632\omega_{20} - 972\omega_{22} + 440\omega_{31} - 20\omega_{33} + 52\omega_{40} + 15\omega_{42})\omega'_{10} \\
& + 31104\omega_{21}\omega'_{20} - 6272\omega_{30}\omega'_{20} + 768\omega_{32}\omega'_{20} - 384\omega_{41}\omega'_{20} - 32256\omega'_{21} \\
& + 116224\omega\omega'_{21} - 31104\omega_{20}\omega'_{21} - 1584\omega_{31}\omega'_{21} + 228\omega_{33}\omega'_{21} + 396\omega_{40}\omega'_{21} \\
& - 171\omega_{42}\omega'_{21} - 14080\omega_{11}\omega'_{30} + 6272\omega_{20}\omega'_{30} - 768\omega_{22}\omega'_{30} + 640\omega_{31}\omega'_{30} \\
& - 32\omega_{40}\omega'_{30} + 1584\omega_{21}\omega'_{31} - 640\omega_{30}\omega'_{31} - 228\omega_{32}\omega'_{31} + 114\omega_{41}\omega'_{31} - 1152\omega'_{32} \\
& - 6272\omega\omega'_{32} - 1584\omega_{11}\omega'_{32} + 768\omega_{20}\omega'_{32} + 228\omega_{31}\omega'_{32} - 57\omega_{40}\omega'_{32} - 96\omega_{21}\omega'_{40} \\
& + 32\omega_{30}\omega'_{40} + 1664\omega\omega'_{41} + 84\omega_{20}\omega'_{41} + 171\omega_{22}\omega'_{41} - 114\omega_{31}\omega'_{41} \\
& - 4\omega_{10}(29056\omega'_{20} - 3520\omega'_{31} + 416\omega'_{40} - 3\omega'_{42}) - 171\omega_{21}\omega'_{42} + 57\omega_{30}\omega'_{42} \\
& - 32\omega\omega'_{43} + 114\omega_{11}\omega'_{43} - 57\omega_{20}\omega'_{43}) \\
& - q^{16}(32(-4608 + 3632\omega_{20} - 972\omega_{22} + 440\omega_{31} - 20\omega_{33} + 52\omega_{40} + 15\omega_{42})\omega'_{10} \\
& + 31104\omega_{21}\omega'_{20} - 6272\omega_{30}\omega'_{20} + 768\omega_{32}\omega'_{20} - 384\omega_{41}\omega'_{20} + 32256\omega'_{21} \\
& + 116224\omega\omega'_{21} - 31104\omega_{20}\omega'_{21} - 1584\omega_{31}\omega'_{21} + 228\omega_{33}\omega'_{21} + 396\omega_{40}\omega'_{21} \\
& - 171\omega_{42}\omega'_{21} - 14080\omega_{11}\omega'_{30} + 6272\omega_{20}\omega'_{30} - 768\omega_{22}\omega'_{30} + 640\omega_{31}\omega'_{30} \\
& - 32\omega_{40}\omega'_{30} + 1584\omega_{21}\omega'_{31} - 640\omega_{30}\omega'_{31} - 228\omega_{32}\omega'_{31} + 114\omega_{41}\omega'_{31} + 1152\omega'_{32} \\
& - 6272\omega\omega'_{32} - 1584\omega_{11}\omega'_{32} + 768\omega_{20}\omega'_{32} + 228\omega_{31}\omega'_{32} - 57\omega_{40}\omega'_{32} - 96\omega_{21}\omega'_{40} \\
& + 32\omega_{30}\omega'_{40} + 1664\omega\omega'_{41} + 84\omega_{20}\omega'_{41} + 171\omega_{22}\omega'_{41} - 114\omega_{31}\omega'_{41} \\
& - 4\omega_{10}(29056\omega'_{20} - 3520\omega'_{31} + 416\omega'_{40} - 3\omega'_{42}) - 171\omega_{21}\omega'_{42} + 57\omega_{30}\omega'_{42} \\
& - 32\omega\omega'_{43} + 114\omega_{11}\omega'_{43} - 57\omega_{20}\omega'_{43})
\end{aligned}$$

$$\begin{aligned}
& + 2q^{14}(16(9216 + 1424\omega_{20} + 1644\omega_{22} - 824\omega_{31} + 20\omega_{33} - 68\omega_{40} - 15\omega_{42})\omega'_{10} \\
& - 26304\omega_{21}\omega'_{20} + 9536\omega_{30}\omega'_{20} - 17152\omega'_{21} + 22784\omega\omega'_{21} + 26304\omega_{20}\omega'_{21} \\
& - 1392\omega_{31}\omega'_{21} + 204\omega_{33}\omega'_{21} + 348\omega_{40}\omega'_{21} - 153\omega_{42}\omega'_{21} + 13184\omega_{11}\omega'_{30} \\
& - 9536\omega_{20}\omega'_{30} - 320\omega_{31}\omega'_{30} + 80\omega_{40}\omega'_{30} + 1392\omega_{21}\omega'_{31} + 320\omega_{30}\omega'_{31} \\
& - 204\omega_{32}\omega'_{31} + 102\omega_{41}\omega'_{31} - 1216\omega'_{32} + 9536\omega\omega'_{32} - 1392\omega_{11}\omega'_{32} + 204\omega_{31}\omega'_{32} \\
& - 51\omega_{40}\omega'_{32} + 240\omega_{21}\omega'_{40} - 80\omega_{30}\omega'_{40} - 128\omega'_{41} - 1088\omega\omega'_{41} - 588\omega_{20}\omega'_{41} \\
& + 153\omega_{22}\omega'_{41} - 102\omega_{31}\omega'_{41} - 4\omega_{10}(5696\omega'_{20} + 3296\omega'_{31} - 272\omega'_{40} - 87\omega'_{42}) \\
& - 153\omega_{21}\omega'_{42} + 51\omega_{30}\omega'_{42} - 64\omega'_{43} + 80\omega\omega'_{43} + 102\omega_{11}\omega'_{43} - 51\omega_{20}\omega'_{43}) \\
& - 2q^8(16(-9216 + 1424\omega_{20} + 1644\omega_{22} - 824\omega_{31} + 20\omega_{33} - 68\omega_{40} - 15\omega_{42})\omega'_{10} \\
& - 26304\omega_{21}\omega'_{20} + 9536\omega_{30}\omega'_{20} + 17152\omega'_{21} + 22784\omega\omega'_{21} + 26304\omega_{20}\omega'_{21} \\
& - 1392\omega_{31}\omega'_{21} + 204\omega_{33}\omega'_{21} + 348\omega_{40}\omega'_{21} - 153\omega_{42}\omega'_{21} + 13184\omega_{11}\omega'_{30} \\
& - 9536\omega_{20}\omega'_{30} - 320\omega_{31}\omega'_{30} + 80\omega_{40}\omega'_{30} + 1392\omega_{21}\omega'_{31} + 320\omega_{30}\omega'_{31} \\
& - 204\omega_{32}\omega'_{31} + 102\omega_{41}\omega'_{31} + 1216\omega'_{32} + 9536\omega\omega'_{32} - 1392\omega_{11}\omega'_{32} + 204\omega_{31}\omega'_{32} \\
& - 51\omega_{40}\omega'_{32} + 240\omega_{21}\omega'_{40} - 80\omega_{30}\omega'_{40} + 128\omega'_{41} - 1088\omega\omega'_{41} - 588\omega_{20}\omega'_{41} \\
& + 153\omega_{22}\omega'_{41} - 102\omega_{31}\omega'_{41} - 4\omega_{10}(5696\omega'_{20} + 3296\omega'_{31} - 272\omega'_{40} - 87\omega'_{42}) \\
& - 153\omega_{21}\omega'_{42} + 51\omega_{30}\omega'_{42} + 64\omega'_{43} + 80\omega\omega'_{43} + 102\omega_{11}\omega'_{43} - 51\omega_{20}\omega'_{43}) \\
& + q^{22}(4\omega_{33}\omega'_{21} - 4\omega_{40}\omega'_{21} - 3\omega_{42}\omega'_{21} - 16\omega_{21}\omega'_{31} - 4\omega_{32}\omega'_{31} + 2\omega_{41}\omega'_{31} \\
& + 16\omega_{11}\omega'_{32} - \omega_{40}\omega'_{32} + 2\omega_{31}(8\omega'_{21} + 2\omega'_{32} - \omega'_{41}) + 4\omega_{20}\omega'_{41} + 3\omega_{22}\omega'_{41} \\
& - 4\omega_{10}\omega'_{42} - 3\omega_{21}\omega'_{42} + \omega_{30}\omega'_{42} + 2\omega_{11}\omega'_{43} - \omega_{20}\omega'_{43}) \\
& - 2q^{10}(32(-2304 + 5208\omega_{20} - 552\omega_{22} - 184\omega_{31} + 52\omega_{33} + 138\omega_{40} - 39\omega_{42})\omega'_{10} \\
& + 17664\omega_{21}\omega'_{20} - 2496\omega_{30}\omega'_{20} + 672\omega_{32}\omega'_{20} - 336\omega_{41}\omega'_{20} - 31872\omega'_{21} \\
& + 166656\omega\omega'_{21} - 17664\omega_{20}\omega'_{21} + 1680\omega_{31}\omega'_{21} - 180\omega_{33}\omega'_{21} - 420\omega_{40}\omega'_{21} \\
& + 135\omega_{42}\omega'_{21} + 5888\omega_{11}\omega'_{30} + 2496\omega_{20}\omega'_{30} - 672\omega_{22}\omega'_{30} - 1664\omega_{31}\omega'_{30} + 528\omega_{40}\omega'_{30} \\
& - 1680\omega_{21}\omega'_{31} + 1664\omega_{30}\omega'_{31} + 180\omega_{32}\omega'_{31} - 90\omega_{41}\omega'_{31} - 1344\omega'_{32} - 2496\omega\omega'_{32} \\
& + 1680\omega_{11}\omega'_{32} + 672\omega_{20}\omega'_{32} - 180\omega_{31}\omega'_{32} + 45\omega_{40}\omega'_{32} + 1584\omega_{21}\omega'_{40} - 528\omega_{30}\omega'_{40} \\
& - 96\omega'_{41} + 4416\omega\omega'_{41} - 828\omega_{20}\omega'_{41} - 135\omega_{22}\omega'_{41} + 90\omega_{31}\omega'_{41} + 135\omega_{21}\omega'_{42} \\
& - 45\omega_{30}\omega'_{42} - 4\omega_{10}(41664\omega'_{20} + 1472\omega'_{31} + 1104\omega'_{40} + 189\omega'_{42}) \\
& - 48\omega'_{43} + 528\omega\omega'_{43} - 90\omega_{11}\omega'_{43} + 45\omega_{20}\omega'_{43})
\end{aligned}$$

$$\begin{aligned}
& + 2q^{12}(32(2304 + 5208\omega_{20} - 552\omega_{22} - 184\omega_{31} + 52\omega_{33} + 138\omega_{40} - 39\omega_{42})\omega'_{10} \\
& + 17664\omega_{21}\omega'_{20} - 2496\omega_{30}\omega'_{20} + 672\omega_{32}\omega'_{20} - 336\omega_{41}\omega'_{20} + 31872\omega'_{21} \\
& + 166656\omega\omega'_{21} - 17664\omega_{20}\omega'_{21} + 1680\omega_{31}\omega'_{21} - 180\omega_{33}\omega'_{21} - 420\omega_{40}\omega'_{21} \\
& + 135\omega_{42}\omega'_{21} + 5888\omega_{11}\omega'_{30} + 2496\omega_{20}\omega'_{30} - 672\omega_{22}\omega'_{30} - 1664\omega_{31}\omega'_{30} \\
& + 528\omega_{40}\omega'_{30} - 1680\omega_{21}\omega'_{31} + 1664\omega_{30}\omega'_{31} + 180\omega_{32}\omega'_{31} - 90\omega_{41}\omega'_{31} \\
& + 1344\omega'_{32} - 2496\omega\omega'_{32} + 1680\omega_{11}\omega'_{32} + 672\omega_{20}\omega'_{32} - 180\omega_{31}\omega'_{32} + 45\omega_{40}\omega'_{32} \\
& + 1584\omega_{21}\omega'_{40} - 528\omega_{30}\omega'_{40} + 96\omega'_{41} + 4416\omega\omega'_{41} - 828\omega_{20}\omega'_{41} - 135\omega_{22}\omega'_{41} \\
& + 90\omega_{31}\omega'_{41} + 135\omega_{21}\omega'_{42} - 45\omega_{30}\omega'_{42} \\
& - 4\omega_{10}(41664\omega'_{20} + 1472\omega'_{31} + 1104\omega'_{40} + 189\omega'_{42}) + 48\omega'_{43} + 528\omega\omega'_{43} \\
& - 90\omega_{11}\omega'_{43} + 45\omega_{20}\omega'_{43}) \\
& + q^2(384\omega_{31}\omega'_{10} + 192\omega_{33}\omega'_{10} + 128\omega_{40}\omega'_{10} - 144\omega_{42}\omega'_{10} + 3584\omega_{10}\omega'_{20} \\
& + 1344\omega_{21}\omega'_{20} - 512\omega_{30}\omega'_{20} + 96\omega_{32}\omega'_{20} - 48\omega_{41}\omega'_{20} + 896\omega'_{21} - 3584\omega\omega'_{21} \\
& - 16\omega_{31}\omega'_{21} - 4\omega_{33}\omega'_{21} + 4\omega_{40}\omega'_{21} + 3\omega_{42}\omega'_{21} - 384\omega_{11}\omega'_{30} - 192\omega_{31}\omega'_{30} \\
& + 64\omega_{40}\omega'_{30} + 384\omega_{10}\omega'_{31} + 16\omega_{21}\omega'_{31} + 192\omega_{30}\omega'_{31} + 4\omega_{32}\omega'_{31} - 2\omega_{41}\omega'_{31} \\
& + 128\omega'_{32} - 512\omega\omega'_{32} - 16\omega_{11}\omega'_{32} - 4\omega_{31}\omega'_{32} + \omega_{40}\omega'_{32} - 128\omega_{10}\omega'_{40} \\
& + 192\omega_{21}\omega'_{40} - 64\omega_{30}\omega'_{40} - 32\omega'_{41} + 128\omega\omega'_{41} + 2\omega_{31}\omega'_{41} \\
& - 3\omega_{22}(448\omega'_{10} + 32\omega'_{30} + \omega'_{41}) - 44\omega_{10}\omega'_{42} \\
& + 3\omega_{21}\omega'_{42} - \omega_{30}\omega'_{42} - 16\omega'_{43} + 64\omega\omega'_{43} - 2\omega_{11}\omega'_{43} \\
& + \omega_{20}(-3584\omega'_{10} - 1344\omega'_{21} + 512\omega'_{30} + 96\omega'_{32} - 148\omega'_{41} + \omega'_{43}))\} \\
& / (2359296\eta^2q^{10}(1 + q^2)^2(-1 - q^4 + q^6 + q^{10}))
\end{aligned}$$

Appendix C

Crossover Temperatures

Here we list all crossover temperatures obtained from our results (T_0) alongside the values given in [67] (\tilde{T}_0), as well as the relative differences $\delta T_0 = \frac{T_0 - \tilde{T}_0}{T_0}$. Values for T_0 are rounded to improve readability.

Table C.1: Crossover temperatures and relative differences for $\Delta = -0.1$

n	T_0	\tilde{T}_0	$ \delta T_0 $
2	4.9664	4.966	$9.0 \cdot 10^{-5}$
3	3.3229	3.323	$3.5 \cdot 10^{-5}$
4	2.5608	2.561	$8.9 \cdot 10^{-5}$
5	2.0729	2.073	$5.8 \cdot 10^{-5}$

Table C.2: Crossover temperatures and relative differences for $\Delta = -0.2$

n	T_0	\tilde{T}_0	$ \delta T_0 $
2	2.4316	2.432	$1.8 \cdot 10^{-4}$
3	1.6433	1.643	$1.9 \cdot 10^{-4}$
4	1.2752	1.275	$1.6 \cdot 10^{-4}$
5	1.0374	1.037	$3.7 \cdot 10^{-4}$

Table C.3: Crossover temperatures and relative differences for $\Delta = -0.3$

n	T_0	\tilde{T}_0	$ \delta T_0 $
2	1.5608	1.561	$1.3 \cdot 10^{-4}$
3	1.0708	1.071	$1.8 \cdot 10^{-4}$
4	0.8392	0.839	$2.0 \cdot 10^{-4}$
5	0.6875	0.687	$6.8 \cdot 10^{-4}$

Table C.4: Crossover temperatures and relative differences for $\Delta = -0.4$

n	T_0	\tilde{T}_0	$ \delta T_0 $
2	1.1029	1.103	$5.9 \cdot 10^{-5}$
3	0.7713	0.771	$3.7 \cdot 10^{-4}$
4	0.6116	0.612	$7.2 \cdot 10^{-4}$
5	0.5054	0.505	$8.5 \cdot 10^{-4}$

Table C.5: Crossover temperatures and relative differences for $\Delta = -0.5$

n	T_0	\tilde{T}_0	$ \delta T_0 $
2	0.8070	0.807	$4.1 \cdot 10^{-5}$
3	0.5777	0.578	$5.0 \cdot 10^{-4}$
4	0.4641	0.464	$2.6 \cdot 10^{-4}$
5	0.3876	0.388	$9.6 \cdot 10^{-4}$

Table C.6: Crossover temperatures and relative differences for $\Delta = -0.6$

n	T_0	\tilde{T}_0	$ \delta T_0 $
2	0.5888	0.589	$3.1 \cdot 10^{-4}$
3	0.4342	0.434	$4.1 \cdot 10^{-4}$
4	0.3540	0.355	$2.7 \cdot 10^{-3}$
5	0.2993	0.300	$2.3 \cdot 10^{-3}$

Table C.7: Crossover temperatures and relative differences for $\Delta = -0.7$

n	T_0	\tilde{T}_0	$ \delta T_0 $
2	0.4128	0.413	$5.0 \cdot 10^{-4}$
3	0.3163	0.318	$5.3 \cdot 10^{-3}$
4	0.2626	0.264	$5.3 \cdot 10^{-3}$
5	0.2252	0.227	$7.9 \cdot 10^{-3}$

Table C.8: Crossover temperatures and relative differences for $\Delta = -0.8$

n	T_0	\tilde{T}_0	$ \delta T_0 $
2	0.2624	0.265	$1.0 \cdot 10^{-2}$
3	0.2114	0.215	$1.7 \cdot 10^{-2}$
4	0.1798	0.184	$2.3 \cdot 10^{-2}$
5	0.1570	0.161	$2.6 \cdot 10^{-2}$

Table C.9: Crossover temperatures and relative differences for $\Delta = -0.9$

n	T_0	\tilde{T}_0	$ \delta T_0 $
2	0.1292	0.137	$6.0 \cdot 10^{-2}$
3	0.1111	0.118	$6.2 \cdot 10^{-2}$
4	0.0981	0.104	$6.1 \cdot 10^{-2}$
5	0.0879	0.092	$4.7 \cdot 10^{-2}$

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