UNIVERSITÄT BONN
Physikalisches Institut

Quantum Spin Models and Extended Conformal Algebras

von
Andreas Honecker

Abstract

First, an algebraic criterion for integrability is discussed –the so-called 'superintegrability'– and some results on the classification of superintegrable quantum spin Hamiltonians based on $sl(2)$ are obtained.
Next, the massive phases of the $\mathbb{Z}_n$-chiral Potts quantum spin chain (a model that violates parity) are studied in detail. It is shown that the excitation spectrum of the massive high-temperature phase can be explained in terms of $n-1$ fundamental quasiparticles. We compute correlation functions from a perturbative and numerical evaluation of the groundstate for the $\mathbb{Z}_3$-chain. In addition to an exponential decay we observe an oscillating contribution. The oscillation length seems to be related to the asymmetry of the dispersion relations. We show that this relation is exact at special values of the parameters for general $\mathbb{Z}_n$ using a form factor expansion.
Finally, we discuss several aspects of extended conformal algebras ($\mathcal{W}$-algebras). We observe an analogy between boundary conditions for $\mathbb{Z}_n$-spin chains and $\mathcal{W}$-algebras and then turn to statements about the structure of $\mathcal{W}$-algebras. In particular, we briefly summarize results on unifying structures present in the space of all quantum $\mathcal{W}$-algebras.

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Für meine Eltern

Ἐπειδὴ τὸ εἰδέναι καὶ τὸ ἐπίστασθαι συμβαίνει περὶ πάσας τὰς μεθόδους, ὧν εἰσὶν ἀρχαὶ ἢ αἴτια ἢ στοιχεῖα, ἐκ τοῦ ταῦτα γνωρίζειν (τότε γὰρ οἰόμεθα γινώσκειν ἕκαστον, ὅταν τὰ αἴτια γνωρίσωμεν τὰ πρῶτα καὶ τὰς ἀρχὰς τὰς πρώτας καὶ μέχρι τῶν στοιχείων), δῆλον ὅτι καὶ τῆς περὶ φύσεως ἐπιστήμης πειρατέον διορίσασθαι πρῶτον τὰ περὶ τὰς ἀρχάς.

ΑΡΙΣΤΟΤΕΛΟΥΣ "ΦΥΣΙΚΗΣ ΑΚΡΟΑΣΕΩΣ." Α. 1.
(Aristoteles' Acht Bücher Physik, 1. Buch, 1.)

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Mathematik und Physik sind die beiden theoretischen Erkenntnisse der Vernunft, welche ihre Objecte a priori bestimmen sollen, die erstere ganz rein, die zweite wenigstens zum Theil rein, dann aber auch nach Massgabe anderer Erkenntnisquellen als der der Vernunft.

Immanuel Kant, Vorrede zur zweiten Auflage der "Kritik der reinen Vernunft"

1. Introduction

Theoretical physicists have paid much attention to low dimensions in the last years. On the one hand, models in low dimensions can more easily be treated also on a mathematically rigorous level, but on the other hand, low dimensions have indeed turned out to be relevant in the description of important experiments. This thesis is centered around two aspects of low-dimensional theoretical physics: $\mathbb{Z}_n$-quantum spin models and extended conformal algebras.

Among the $\mathbb{Z}_n$-quantum spin models we will mainly concentrate on a '$\mathbb{Z}_n$-chiral Potts model'. The first chiral Potts model that was introduced in 1981 by Ostlund in order to describe incommensurate phases of physisorbed systems [114] was a classical 2D spin model. The associated quantum chain Hamiltonians were obtained in 1981-82 by Rittenberg et al. [108, 39]. Because this chain was not self-dual the location of the critical manifold was difficult. In 1983, Howes, Kadanoff and den Nijs introduced a self-dual $\mathbb{Z}_3$-symmetric chiral quantum chain [97], which however, does not correspond to a two-dimensional model with positive Boltzmann weights. Soon afterwards, von Gehlen and Rittenberg noticed that the remarkable property of the first gap of this model being linear in the inverse temperature also applies to the second gap and can be generalized to arbitrary $\mathbb{Z}_n$ [70]. Furthermore, the authors of [70] showed that the Ising-like form of the eigenvalues is related to this $\mathbb{Z}_n$-Hamiltonian satisfying the Dolan-Grady integrability condition [45] which is equivalent [115, 42, 43] to Onsager's algebra [113]. It was then shown by Au-Yang, Baxter, McCoy, Perk et al. that this integrability property – nowadays called 'superintegrability' – can be implemented in a 2D classical model with Boltzmann weights defined on higher genus Riemann surfaces that satisfy a generalized Yang-Baxter relation. In the sequel the chiral Potts model attracted much attention because of these mathematical aspects, i.e. on the one hand due to the generalized Yang-Baxter relations [4, 5, 6, 10, 11, 12, 21, 22, 109, 110, 119, 121] and on the other hand because of Onsager's algebra [42, 43, 120, 1]. We will present new results showing that the model is also 'physically' very interesting although it is not directly related to a realistic 2D physisorbed system.

We start by a general discussion of quantum spin models and indicate how one might systematically construct integrable nearest neighbour interaction quantum spin models exclusively by algebraic means. Afterwards, we specialize to $\mathbb{Z}_n$-quantum spin chains but drop the requirement of integrability.

One of our main interests will be the excitation spectrum of $\mathbb{Z}_n$-quantum spin chains. We will show that in the massive phases the excitation spectrum can be explained in terms of quasiparticles. Although this is not very surprising, a particle interpretation is not directly incorporated into the spin chain Hamiltonian. Therefore it was not recognized until very recently that a quasiparticle interpretation of the complete excitation spectrum is possible. Using numerical techniques we were able to show that the low-lying excitations in the zero momentum sectors can be explained in terms of $n-1$ fundamental particles for $n = 3$, 4 at general values of the parameters [68, 66] and checked for $n = 3$ that this quasiparticle picture extends to general momenta [69]. For the superintegrable $\mathbb{Z}_3$-chiral Potts model McCoy et al. have derived a quasiparticle picture of the complete spectrum using techniques related to the Bethe ansatz [41]. Recently, they argued that this quasiparticle picture should in general be valid for the integrable $\mathbb{Z}_3$-chiral Potts quantum chain [103]. In this thesis we will show that both results can be combined into the general statement that the massive high-temperature phases of general $\mathbb{Z}_n$ spin quantum chains have quasiparticle spectra. In fact, this quasiparticle picture will in certain cases give small corrections to the additivity of energy in the momentum zero sectors observed in [68].

Another main issue will be correlation functions of the $\mathbb{Z}_n$-chiral Potts model. Since a scaling exponent for the wave vector in the low-temperature phase of the $\mathbb{Z}_3$-chiral Potts model has been calculated in [105, 66] from level crossings in the ground state one expects an oscillatory contribution to the correlation functions also in the massive phases. We will demonstrate the presence of this oscillation by computing low- and high-temperature series and numerical evaluation of the ground state. These computations are limited to short distances. Therefore we also use a form factor expansion for the correlation functions which leads to a better conceptual understanding of the oscillation.

These $\mathbb{Z}_n$-spin quantum chains have conformally invariant second order phase transitions for particular values of the parameters. They can be described by rational models of $\mathbb{Z}_n$ parafermions [56] with $c > 1$ (for $n > 4$). The $\mathbb{Z}_n$ parafermion algebras have the disadvantage that they are non-local and that each algebra only describes precisely one rational conformal field theory. However, Virasoro-minimal models have $c < 1$ [24] and are therefore not useful for describing these second order phase transitions. The discovery of extended conformal algebras [129] (also called $\mathcal{W}$-algebras – for a review see e.g. [33]) was a major simplification because these algebras are local and –like the Virasoro algebra– admit infinite series of minimal models. Nowadays the second order phase transitions of $\mathbb{Z}_n$-spin chains can conveniently be described by the first unitary minimal models of the so-called $\mathcal{WA}_{n-1}$-algebras [8, 57, 54, 55]. Similarly, one also needs $c > 1$ for applications in string theory. Very important applications require $N = 2$ supersymmetric rational conformal fields theories with $c = 9$ (see e.g. [75, 76]). Consequently, the classification of all rational conformal field theories is a natural question. Since those with $c > 1$ are obtained from $\mathcal{W}$-algebras one may expect that $\mathcal{W}$-algebras play an important rôle in this classification program. Another motivation for the study of $\mathcal{W}$-algebras is that $\mathcal{W}$-algebras have a rich mathematical structure, their complete classification still being an open question.

With this thesis we will also try to contribute to these issues. Once again, we will look at the aforementioned second order phase transitions from the point of view of representations of $\mathcal{W}$-algebras with non-trivial boundary conditions. We then turn to questions relevant for the classification problem. The classical versions of $\mathcal{W}$-algebras are (to some extent) more easy to handle. We will therefore use them to examine cosets and orbifolds after addressing some basic problems of covariance with respect to the Virasoro subalgebra of the classical $\mathcal{W}$-algebra. Some puzzles (see e.g. [51]) and also some confusion concerning the structure of quantum $\mathcal{W}$-algebras have recently been explained with the concept of 'unifying $\mathcal{W}$-algebras' [27, 28]. We summarize these results and discuss their relevance for the classification problem.

Perturbations of conformal field theories (see e.g. [111]) describe the off-critical scaling region in statistical mechanics. For the $\mathbb{Z}_n$-chiral Potts models two types of perturbations are relevant: A thermal perturbation (see e.g. [130, 131, 132, 111]) that makes the models massive and a chiral perturbation [38] that breaks parity. Both perturbations separately are integrable but it is still an open question if the combined perturbation is also integrable. $\mathcal{W}$-algebras might also be useful for addressing problems of this type which is however beyond the scope of this thesis.

The outline of this thesis is as follows. Chapter 2 contains a review of the algebraic formulation of superintegrability and indicates how superintegrable quantum spin models can be constructed systematically. In chapter 3 we summarize basic facts about the chiral Potts model and perturbation series. In particular, in section 3.2 we present a precise duality statement. Then, the excitation spectrum of $\mathbb{Z}_n$-spin chains is examined in chapter 4. After reviewing the quasiparticle picture for the superintegrable $\mathbb{Z}_3$-chiral Potts model [41] we start by studying the low-lying levels with high- and low-temperature series. These results illustrate a general quasiparticle picture which we discuss in section 4.4. This quasiparticle picture is strictly valid only in the infinite lattice limit but we also discuss finite-size corrections. Since we use perturbative arguments for the derivation of this quasiparticle picture we also have to discuss the radius of convergence in section 4.5. The various aspects of the correlation functions mentioned above are discussed in chapter 5.

The final chapter 6 shifts to a different aspect of low-dimensional theoretical physics: Extended conformal algebras. In section 6.2 we show how automorphisms of Casimir $\mathcal{W}$-algebras can be used to find extensions of rational conformal field theories by imposing twisted boundary conditions. The relevance of these results to $\mathbb{Z}_n$-quantum spin chains is discussed in section 6.3. We then turn to classical $\mathcal{W}$-algebras in section 6.4 and discuss their $su(1,1)$ structure. For classical $\mathcal{W}$-algebras one can get a good handle on orbifolds and cosets as we show in section 6.5. These results are useful also for obtaining new insights in the structure of quantum $\mathcal{W}$-algebras. Some new statements about the space of quantum $\mathcal{W}$-algebras are summarized in section 6.6 where in particular the notion of 'unifying $\mathcal{W}$-algebras' is explained.

This thesis is (to a large extent) a summary of already published material. More precisely, the following sections are based on the following publications:

Sections 3.2., 4.3. and 5.3.:
: N.S. Han, A. Honecker, *Low-Temperature Expansions and Correlation Functions of the $\mathbb{Z}_3$-Chiral Potts Model*, J. Phys. A: Math. Gen. **27** (1994) p. 9

Section 4.2.:
: G. von Gehlen, A. Honecker, *Multi-Particle Structure in the $\mathbb{Z}_n$-Chiral Potts Models*, J. Phys. A: Math. Gen. **26** (1993) p. 1275

Sections 4.2., 4.4., 4.5., 5.1., 5.4. and appendices A, B:
: A. Honecker, *A Perturbative Approach to the Chiral Potts Model*, preprint BONN-TH-94-21, hep-th/9409122

Section 5.2.:
: G. von Gehlen, A. Honecker, *Excitation Spectrum and Correlation Functions of the $\mathbb{Z}_3$-Chiral Potts Quantum Spin Chain*, Nucl. Phys. **B435** (1995) p. 505

Sections 6.2. and 6.3.:
: A. Honecker, *Automorphisms of $\mathcal{W}$-Algebras and Extended Rational Conformal Field Theories*, Nucl. Phys. **B400** (1993) p. 574

Section 6.5.:
: J. de Boer, A. Honecker, L. Fehér, *A Class of $\mathcal{W}$-Algebras with Infinitely Generated Classical Limit*, Nucl. Phys. **B420** (1994) p. 409

Section 6.6.:
: R. Blumenhagen, W. Eholzer, A. Honecker, K. Hornfeck, R. Hübel, *Unifying $\mathcal{W}$-Algebras*, Phys. Lett. **B332** (1994) p. 51
: R. Blumenhagen, W. Eholzer, A. Honecker, K. Hornfeck, R. Hübel, *Coset Realization of Unifying $\mathcal{W}$-Algebras*, preprint BONN-TH-94-11, DFTT-25/94, hep-th/9406203, to appear in Int. Jour. of Mod. Phys. **A**

There are some minor extensions throughout these sections. The previously unpublished material is concentrated mainly in sections 2.2. – 2.4. and section 6.4.

I was at the mathematical school, where the master taught his pupils after a method scarce imaginable to us in Europe. The proposition and demonstration were fairly written on a thin wafer, with ink composed of a cephalic tincture. This the student was to swallow upon a fasting stomach, and for three days following eat nothing but bread and water. As the wafer digested the tincture mounted to the brain, bearing the proposition along with it.

Jonathan Swift in "Gulliver's Travels"

2. Superintegrable quantum spin models

By now an abundance of integrable classical spin models in two space dimensions, or equivalently quantum spin chains in one space dimension, are known. The quantum spin chain Hamiltonians in turn can be regarded as evolution operators of a lattice field theory in one plus one dimensions. This indicates that it would be desirable to know also integrable spin models in higher dimensions in order not to be restricted to surface physics or other planar media. Unfortunately, very little is known so far about higher dimensions despite major efforts.

A promising idea was put forward in [45] using some algebraic criterion for a particular kind of integrability – the so-called 'superintegrability'. To our knowledge, no results in dimensions greater than one have been obtained with this criterion yet either. In this section we would like to give some indications how one can systematically construct superintegrable quantum spin Hamiltonians. So far, we have not yet reached the goal of finding integrable models in higher dimensions. Nevertheless we show that the problem is in principle amenable to computer computation and we also obtain a few related new results [1]).

2.1. The general setting

Def. I: (Nearest neighbour interaction quantum spin model) Let Λ be a lattice of dimension d and $\mathcal{F}$ be its fundamental domain. Furthermore, consider an associative algebra of dimension n with generators Ω^i including the identity $\mathbb{1}$. For any finite subset $S(\Lambda) \subset \Lambda$ with p points define operators $\Omega^i_{\vec{x}}$ associated to 'site' $\vec{x} \in S(\Lambda)$ by operators $\mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes \Omega^i \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1}$ in the p-fold tensor product of the algebra with itself. Then, a general nearest neighbour interaction quantum spin Hamiltonian in d dimensions is given by

$$H^{(\mathrm{general})} = \sum_{\vec{x}\in S(\Lambda)} \sum_{i=1}^{n} d_i \Omega^i_{\vec{x}} + \lambda \sum_{\vec{x}\in S(\Lambda)} \sum_{\vec{e}\in\mathcal{F}} \sum_{i=1}^{n} \sum_{j=1}^{n} v^{\vec{e}}_{i,j} \Omega^i_{\vec{x}} \Omega^j_{\vec{x}+\vec{e}} \,. \qquad (2.1.1)$$

A Hamiltonian of this type is called '*isotropic*' if the coupling constants $v^{\vec{e}}_{i,j}$ do not depend on the direction $\vec{e}$ of the interaction, i.e. $v^{\vec{e}}_{i,j} = v_{i,j}$ for all $\vec{e}$.

The Hamiltonian (2.1.1) is of the form

$$H = H_0 + \lambda V \,. \qquad (2.1.2)$$

[1]) Note that recently a different algebraic approach to the construction of integrable quantum spin models in one dimension has been proposed in [81].

It was shown in [45, 42, 43] that Hamiltonians of this form are integrable if

$$[H_0,[H_0,[H_0,V]]] = c_1[H_0,V]\,, \tag{2.1.3a}$$

$$[V,[V,[V,H_0]]] = c_2[V,H_0]\,. \tag{2.1.3b}$$

We will call a Hamiltonian of type (2.1.2) satisfying (2.1.3) '*superintegrable*' (note that this terminology is not used entirely consistent in the literature – in contrast to us, some authors include the generalized Yang-Baxter relations in the notion of superintegrability).

Clearly, one can modify c_1 and c_2 by rescaling the individual terms H_0 and V of the Hamiltonian. This is usually exploited in order to set $c_1 = c_2 = 16$. However, we will not impose this normalization condition but will instead normalize H_0 and V suitably. One should keep in mind that if $H_0 + \lambda V$ is superintegrable, so is $(hH_0) + \lambda(vV)$ for arbitrary h, v.

The condition (2.1.3) is trivially satisfied if $[H_0, V] = 0$. In this case, one can simultaneously diagonalize H_0 and V and in this manner diagonalize H for general λ. Clearly, for $[H_0, V] = 0$ all eigenvalues of H are linear in λ. Therefore, if λ should play the rôle of temperature, the Hamiltonian $H = H_0 + \lambda V$ gives rise to trivial thermodynamics. Thus, the non-trivial physics must be given by the potential, usually for $\lambda \to \infty$, i.e. the physically relevant Hamiltonian is $H = V + \hat{\lambda} H_0$ with small $\hat{\lambda}$. In this case the diagonalization of V may still be a difficult task although the conservation of H_0 can be very helpful.

For $[H_0, V] \neq 0$ one can recursively generate Onsager's algebra [113] from $A_0 = H_0$ and $A_1 = V$ (see [45, 42, 43]):

$$[A_m, A_n] = 4G_{m-n}\,, \qquad [G_m, A_n] = 2A_{n+m} - 2A_{n-m}\,, \qquad [G_m, G_n] = 0 \tag{2.1.4}$$

if (2.1.3) is satisfied with $c_1 = c_2 = 16$. From (2.1.4) one obtains the following infinite set of conserved commuting charges:

$$-Q_m = \frac{1}{2}\left(A_m + A_{-m} + \lambda A_{m+1} + \lambda A_{-m+1}\right)\,. \tag{2.1.5}$$

Note that $G_{-1} = -G_1 = \frac{1}{4}[H_0, V]$. Thus, if $[H_0, V] = 0$ the recurrence relations (2.1.4) can be trivially solved leading to $A_m = A_n$ if $m \equiv n \bmod 2$. In this case, one has $Q_m = Q_n$ for $m \equiv n \bmod 2$, i.e. the Hamiltonian is not necessarily integrable in the sense that it has an infinite set of conserved commuting charges. This motivates the following definitions:

Def. II: A Hamiltonian of the form (2.1.2) is called '*quasi superintegrable*' if it satisfies $[H_0, V] = 0$.
Def. III: A Hamiltonian satisfying (2.1.3) with $[H_0, V] \neq 0$ is called '*strictly superintegrable*'.

2.2. First considerations

We will be interested in associative algebras that have finite dimensional (complex) defining representations. These algebras can be considered as subalgebras of $gl(n, \mathbb{C})$ for some n. In the Hamiltonian (2.1.1) we may restrict to operators $\Omega^i \in sl(n, \mathbb{C})$ for the following reason:

The complement of $sl(n,\mathbb{C})$ in $gl(n,\mathbb{C})$ is spanned by the identity $\mathbb{1}$. If the identity $\mathbb{1}$ should appear in the potential term V, this part of the potential could be absorbed in the free part H_0. Now, if the identity would appear in the free part H_0 it would shift the ground state energy per site e_0 by a constant amount and not change the excitation spectrum. Such a modification may be neglected because of its physical irrelevance. Thus, we assume $\Omega^i \in sl(n,\mathbb{C})$ in (2.1.1).

Next we note that the conditions (2.1.3) are local ones. We may therefore choose a suitable domain $S(\Lambda)$ and suitable boundary conditions. Furthermore note that the eigenvalues of the Hamiltonian (2.1.1) will not depend on the details of the lattice Λ but only on the way how neighbours are linked. We will therefore restrict to cubic lattices in d dimensions. This leads us to the following specialization of the Hamiltonian (2.1.1):

$$H^{(\text{general}')} = \sum_{\substack{\vec{x}\in\mathbb{Z}^d \\ 1\leq x_i\leq N_i}} \sum_{i=1}^{n^2-1} d_i \Omega^i_{\vec{x}} + \lambda \sum_{\substack{\vec{x}\in\mathbb{Z}^d \\ 1\leq x_i\leq N_i}} \sum_{i=1}^{d} \sum_{a=1}^{n^2-1} \sum_{b=1}^{n^2-1} v^i_{a,b} \Omega^a_{\vec{x}} \Omega^b_{\vec{x}+\vec{e}_i} \tag{2.2.1}$$

where n is now the dimension of the defining representation of $sl(n,\mathbb{C})$. On (2.2.1) we will impose periodic boundary conditions, i.e. the x_i will be identified if they are equal mod N_i.

Finally we make some observations that will be useful for treating the problem on the computer. For a Hamiltonian of type (2.1.1) the conditions (2.1.3) will involve at most four-fold products of generators $\Omega^i_{\vec{x}}$ sitting on four neighbouring sites. Due to the locality of the conditions (2.1.3) this means that we may choose all $N_i = 4$ when checking them for a general ansatz of the form (2.2.1).

Note that the condition $[H_0, V] = 0$ does not involve the dimensionality of the lattice. Therefore, for any solution $\{d_i, v_{a,b}\}$ with $[H_0, V] = 0$ in $d = 1$ we immediately obtain the corresponding general solution in arbitrary dimensions d by fixing the parameters $\{d_i, v^j_{a,b}\}$ such that for fixed j they satisfy the equations for $d = 1$ independently.

After these first general considerations the problem of solving (2.1.3) is now straightforward although not necessarily very easy.

2.3. The quasi superintegrable case

As we have pointed out before we are mainly interested in strictly superintegrable spin chain Hamiltonians. However, in order to single them out among all solutions to (2.1.3) we have to find the quasi superintegrable ones first.

Fortunately, this problem is comparably simple. In order to evaluate $[H_0, V]$ for a Hamiltonian of the form (2.2.1) we do in fact not need that the Ω^a form an associative algebra, we need nothing else than the Lie bracket. Introducing structure constants by

$$[\Omega^a, \Omega^b] = \sum_c f^{ab}_c \Omega^c \tag{2.3.1}$$

one obtains

$$[H_0, V] = \sum_{\substack{\vec{x}\in\mathbb{Z}^d \\ 1\leq x_i\leq N_i}} \sum_{i=1}^{d} \sum_{a,b,c,d=1}^{n^2-1} d_a \left\{ v^i_{b,c} f^{ab}_d + v^i_{d,b} f^{ab}_c \right\} \Omega^d_{\vec{x}} \Omega^c_{\vec{x}+\vec{e}_i} . \tag{2.3.2}$$

Clearly, $H_0 + \lambda V$ will be quasi superintegrable iff

$$\sum_{a,b=1}^{n^2-1} d_a \left\{ v^i_{b,c} f^{ab}_d + v^i_{d,b} f^{ab}_c \right\} = 0 \qquad \forall c,\, d,\, i\,. \tag{2.3.3}$$

The condition (2.3.3) is very reminiscent of an invariance condition with respect to the generators of the Lie algebra for which $d_a \neq 0$. Thus, it will not be surprising if the quasi superintegrable spin chain Hamiltonians turn out to have extra continuous symmetries.

2.4. Results

In this section we will present some new results for quantum spin models based on $sl(2,\mathbb{C})$ and afterwards recall some facts about $\mathbb{Z}_n$ spin chains. After complexification $sl(2,\mathbb{C})$ is the same as $su(2)$. We can therefore use the standard Pauli spin matrices

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{2.4.1}$$

In fact, we will not need the matrix realization given by (2.4.1). Instead we will look at the associative algebra generated by $\mathbb{1}$, σ^z, σ^x, σ^y, e.g. $(\sigma^z)^2 = (\sigma^x)^2 = (\sigma^y)^2 = \mathbb{1}$.

In the basis (2.4.1) the isotropic Ising quantum spin model on a cubic lattice in d dimensions which is one special case of (2.2.1) is given by:

$$H^{(\mathrm{Ising})} = - \sum_{\substack{\vec{x}\in\mathbb{Z}^d \\ 1\leq x_i\leq N_i}} \sigma^z_{\vec{x}} - \lambda \sum_{\substack{\vec{x}\in\mathbb{Z}^d \\ 1\leq x_i\leq N_i}} \sum_{i=1}^{d} \sigma^x_{\vec{x}} \sigma^x_{\vec{x}+\vec{e}_i} . \tag{2.4.2}$$

Note that superintegrability is known since Onsager's days for $H^{(\mathrm{Ising})}$ only in $d=1$. For $d=2$ we will show below that $H^{(\mathrm{Ising})}$ is not superintegrable.

Let us now turn to the most general ansatz for a nearest neighbour interaction Hamiltonian based on $sl(2,\mathbb{C})$ in d dimensions. In addition to the previous comments we recall that $SO(3)$ acts on $su(2)$ by inner conjugations. This can be exploited in order to fix the basis in $sl(2,\mathbb{C})$ and the normalization of H_0 such that $H_0 = -\sum_{\vec{x}} \sigma^z_{\vec{x}}$. Thus, the general spin-1/2 Hamiltonian becomes

$$H = - \sum_{\substack{\vec{x}\in\mathbb{Z}^d \\ 1\leq x_i\leq N_i}} \sigma^z_{\vec{x}} - \lambda \sum_{\substack{\vec{x}\in\mathbb{Z}^d \\ 1\leq x_i\leq N_i}} \sum_{i=1}^{d} \sum_{a=0}^{2} \sum_{b=0}^{2} v^i_{a,b} \Omega^a_{\vec{x}} \Omega^b_{\vec{x}+\vec{e}_i} \tag{2.4.3}$$

with $\Omega^0 = \sigma^z$, $\Omega^1 = \sigma^x$ and $\Omega^2 = \sigma^y$. Note that there may be some residual freedom of choice of basis corresponding to rotations around the z-axis.

First we consider one-dimensional models. In $d = 1$ the general ansatz (2.4.3) becomes

$$H = -\sum_{x=1}^{N} \sigma_x^z - \lambda \sum_{x=1}^{N} \sum_{a=0}^{2} \sum_{b=0}^{2} v_{a,b} \Omega_x^a \Omega_{x+1}^b \tag{2.4.4}$$

With this ansatz one can show by a tedious but straightforward calculation that there are only two different inequivalent families of solutions to eq. (2.1.3) given by theorems I and II.

Theorem I: *The most general quasi superintegrable Hamiltonian of type (2.4.4) in $d = 1$ is given by:*

$$H^{(1)} = -\sum_{x=1}^{N} \sigma_x^z - \lambda \sum_{x=1}^{N} \left\{ \sigma_x^x \sigma_{x+1}^x + \sigma_x^y \sigma_{x+1}^y + \hat{v} \left(\sigma_x^x \sigma_{x+1}^y - \sigma_x^y \sigma_{x+1}^x \right) + \tilde{v} \sigma_x^z \sigma_{x+1}^z \right\} . \tag{2.4.5}$$

■

Remarks:

1) The Hamiltonian (2.4.5) is invariant with respect to rotations in the two-dimensional space spanned by σ^x, σ^y. For $\hat{v} = \tilde{v} = 0$ this solution contains the Hamiltonian generated by [1] with (in the notations of [1]) $g_1 = g_{-1}$. Note that the Hamiltonian eq. (11) of [1] is *not* superintegrable for general $g_1 \neq g_{-1}$.
2) In [79] a spin-1 Hamiltonian of the type $H = \sum_x \vec{S}_x \cdot \vec{S}_{x+1}$ was studied numerically for up to 22 sites. This Hamiltonian is a special case of (2.4.5) and demonstrates the usefulness of conservation of H_0 for numerical computations.

The second solution to (2.1.3) is strictly superintegrable. For the second solution in $d = 1$ we have some freedom of rotation between σ^x and σ^y. After fixing this freedom we arrive at

Theorem II: *The most general strictly superintegrable Hamiltonian of type (2.4.4) in $d = 1$ is given by:*

$$H^{(2)} = -\sum_{x=1}^{N} \sigma_x^z - \lambda \sum_{x=1}^{N} \left\{ \sigma_x^x \sigma_{x+1}^x + v \left(\sigma_x^x \sigma_{x+1}^y - \sigma_x^y \sigma_{x+1}^x \right) \right\} . \tag{2.4.6}$$

■

Remark: The solution (2.4.6) contains the Ising model (2.4.2) in $d = 1$ for $v = 0$.

The conditions for a general Hamiltonian (2.4.3) to be superintegrable are already very complicated for spin 1/2 in $d = 1$. Therefore, it does not make sense to start with a general ansatz in $d > 1$ but one has to restrict oneself to special cases.

A trivial d-dimensional strictly superintegrable Hamiltonian can be obtained from (2.4.6) by setting all $v_{a,b}^i = 0$ for $i \neq k$ with some fixed k. For $v_{a,b}^k$ one then simply takes the solution (2.4.6). However, this solution is trivial since it consists of decoupled one dimensional models. Therefore, we will not consider solutions of this type any more.

First, we note that the Hamiltonian $H^{(\mathrm{Ising})}$ given by eq. (2.4.2) is *not* superintegrable in $d=2$. Even more strongly, one can show that

Theorem III: *There is no strictly superintegrable $\mathbb{Z}_2$ charge conserving Hamiltonian of type (2.4.3) in $d=2$. Here $\mathbb{Z}_2$ charge conservation means that $v^i_{0,1} = v^i_{0,2} = v^i_{1,0} = v^i_{2,0} = 0$ for $i=1,\,2$.* ■

However, from the preceding discussions we obtain the

Corollary: The Hamiltonian

$$H^{(1,d)} = -\sum_{\substack{\vec{x}\in\mathbb{Z}^d \\ 1\le x_i\le N_i}} \sigma^z_{\vec{x}} - \lambda \sum_{\substack{\vec{x}\in\mathbb{Z}^d \\ 1\le x_i\le N_i}} \sum_{i=1}^{d} \Big\{ v_i \left(\sigma^x_{\vec{x}}\sigma^x_{\vec{x}+\vec{e}_i} + \sigma^y_{\vec{x}}\sigma^y_{\vec{x}+\vec{e}_i}\right) + \hat{v}_i \left(\sigma^x_{\vec{x}}\sigma^y_{\vec{x}+\vec{e}_i} - \sigma^y_{\vec{x}}\sigma^x_{\vec{x}+\vec{e}_i}\right) + \tilde{v}_i \sigma^z_{\vec{x}}\sigma^z_{\vec{x}+\vec{e}_i} \Big\} \tag{2.4.7}$$

is quasi superintegrable for general d.

Current knowledge about strictly superintegrable spin quantum chains based on $sl(n)$ with $n>2$ is restricted to the result of von Gehlen and Rittenberg who constructed the so-called '*superintegrable $\mathbb{Z}_n$-chiral Potts model*' [70]. More precisely, one has

Theorem IV: *([70]) The $\mathbb{Z}_n$-chiral Potts spin quantum chain defined by*

$$H^{(n)}_N = -\sum_{j=1}^{N} \left(2\mathsf{H}_j + \lambda \sum_{k=1}^{n-1} \left(1 - i\cot\frac{\pi k}{n}\right) \Gamma^k_j \Gamma^{n-k}_{j+1} \right) \tag{2.4.8}$$

is strictly superintegrable. H and Γ are operators in the fundamental representation of $sl(n)$. H is the Cartan generator of the principal $sl(2)$, i.e. $\mathsf{H} = \mathrm{diag}\left(\frac{n-1}{2}, \ldots, -\frac{n-1}{2}\right)$. Furthermore, one has $\Gamma = \left(\sum_\alpha E_\alpha\right) + E_{-\gamma}$ where the sum runs over the $n-1$ simple positive roots and γ is the highest root. E_β is the root vector associated to a root β in a normalization such that E_α for a simple root α has a single non-zero entry equal to one on the first upper off-diagonal. ■

Ahn and Shigemoto [1] realized that one can add terms of type $\frac{1}{2} g_l \left(A_{m+l} + A_{-m+l}\right)$ with arbitrary parameters g_l to the conserved charges Q_m in (2.1.5), still ensuring the commutativity of these charges. Furthermore, $A_{-1} = V - \frac{1}{2}[H_0, V]$ is obviously still a nearest neighbour interaction for Hamiltonians of type (2.1.1). Thus, adding $\frac{1}{2}\hat{\lambda}\left(A_{m-1} + A_{-m-1}\right)$ to (2.1.5) they arrived at the following corollary to theorem IV:

Corollary: ([1]) The $\mathbb{Z}_n$-spin quantum chain defined by

$$H^{(n)}_N = -\sum_{j=1}^{N} \left[2\mathsf{H}_j + \sum_{k=1}^{n-1} \left(1 - i\cot\frac{\pi k}{n}\right) \left(\lambda \Gamma^k_j \Gamma^{n-k}_{j+1} + \hat{\lambda} \Xi^k_j \Xi^{n-k}_{j+1}\right) \right] \tag{2.4.9}$$

is integrable for general λ, $\hat{\lambda}$, i.e. it gives rise to an infinite set of commuting charges. The additional operator Ξ is defined by $\Xi = \left(\sum_\alpha E_\alpha\right) - E_{-\gamma}$.

Remark: The Hamiltonian (2.4.9) is neither quasi nor strictly superintegrable for general values of the parameters.

Einstweilen wissen wir noch gar nicht, in welcher Sprache wir über das Geschehen im Atom reden können. Wir haben zwar eine mathematische Sprache, das heißt ein mathematisches Schema, mit Hilfe dessen wir die stationären Zustände des Atoms oder Übergangswahrscheinlichkeiten von einem Zustand zu einem anderen ausrechnen können. Aber wir wissen noch nicht – wenigstens noch nicht allgemein – wie diese Sprache mit der gewöhnlichen Sprache zusammenhängt.

Werner Heisenberg in "Der Teil und das Ganze", Kapitel zu 1925-1926

3. The chiral Potts quantum chain

This chapter and chapters 4 and 5 of this thesis focus on the '$\mathbb{Z}_n$-chiral Potts quantum chain' which is a generalization of (2.4.8). From here on we will rely on methods that do not make use of any particular integrability properties.

3.1. Preliminaries

This section summarizes well-known basic facts about $\mathbb{Z}_n$-spin quantum chains. We also introduce some notions that will be useful later on. For more details see e.g. the review [40].

In the following we will study the $\mathbb{Z}_n$-spin quantum chain with N sites which is defined by the Hamiltonian:

$$H_N^{(n)} = -\sum_{j=1}^{N}\sum_{k=1}^{n-1}\left\{\bar{\alpha}_k \sigma_j^k + \lambda \alpha_k \Gamma_j^k \Gamma_{j+1}^{n-k}\right\}. \tag{3.1.1}$$

For the low-temperature phase (large λ) it is more convenient to use a different normalization than (3.1.1):

$$\tilde{H}_N^{(n)} = \tilde{\lambda} H_N^{(n)} = -\sum_{j=1}^{N}\sum_{k=1}^{n-1}\left\{\tilde{\lambda}\bar{\alpha}_k \sigma_j^k + \alpha_k \Gamma_j^k \Gamma_{j+1}^{n-k}\right\} \tag{3.1.2}$$

with $\tilde{\lambda} = \lambda^{-1}$.

σ_j and Γ_j freely generate a finite dimensional associative algebra with involution by the following relations ($1 \leq j, l \leq N$):

$$\begin{gathered} \sigma_j\sigma_l = \sigma_l\sigma_j\,, \qquad \Gamma_j\Gamma_l = \Gamma_l\Gamma_j\,, \qquad \sigma_j\Gamma_l = \Gamma_l\sigma_j\omega^{\delta_{j,l}}\,, \qquad \sigma_j^n = \Gamma_j^n = \mathbb{1}\,, \\ \sigma_j^+ = \sigma_n^{n-1}\,, \qquad \Gamma_j^+ = \Gamma_j^{n-1} \end{gathered} \tag{3.1.3}$$

where ω is the primitive nth root of unity $\omega = e^{\frac{2\pi i}{n}}$.

For the Hamiltonian (3.1.1) we also have to specify boundary conditions, i.e. we have to define Γ_{N+1}. The following choices will be considered (in the terminology we follow Cardy [37]):

1) *Free* boundary conditions

$$\Gamma_{N+1} = 0\,. \tag{3.1.4a}$$

2) *Toroidal* boundary conditions, i.e. we identify the $N+1$st site with the 1st site.

a) *Cyclic* boundary conditions

$$\Gamma_{N+1} = \omega^{-R}\Gamma_1 \,. \tag{3.1.4b}$$

b) *Periodic* boundary conditions which are the $R = 0$ special case of cyclic boundary conditions

$$\Gamma_{N+1} = \Gamma_1 \,. \tag{3.1.4c}$$

c) *Twisted* boundary conditions

$$\Gamma_{N+1} = \omega^{-R}\Gamma_1^+ \,. \tag{3.1.4d}$$

We will mainly focus on periodic boundary conditions.

The Hamiltonian (3.1.1) contains $2n-1$ parameters: The temperature-like parameter λ that we choose to be real and the complex constants $\bar{\alpha}_k$ and α_k. $H_N^{(n)}$ is hermitean iff $\bar{\alpha}_k = \bar{\alpha}_{n-k}^*$ and $\alpha_k = \alpha_{n-k}^*$.

The algebra (3.1.3) is conveniently represented in

$$\mathcal{H}_N := \underbrace{\mathbb{C}^n \otimes \mathbb{C}^n \otimes \ldots \otimes \mathbb{C}^n}_{N \text{ times}} \tag{3.1.5}$$

labeling the standard basis of $\mathbb{C}^n$ by $\{e_0, \ldots, e_{n-1}\}$. Then a basis for (3.1.5) is given by:

$$|\, i_1 \ldots i_N \rangle := e_{i_1} \otimes \ldots \otimes e_{i_N} \,, \qquad 0 \leq i_j \leq n-1. \tag{3.1.6}$$

Now the following operation in the space (3.1.5) is a faithful irreducible representation r of the algebra (3.1.3):

$$\begin{aligned} r(\sigma_j)\,|\, i_1 \ldots i_j \ldots i_N \rangle &= \omega^{i_j} \,|\, i_1 \ldots i_j \ldots i_N \rangle \,, \\ r(\Gamma_j)\,|\, i_1 \ldots i_j \ldots i_N \rangle &= |\, i_1 \ldots (i_j + 1 \bmod n) \ldots i_N \rangle \,. \end{aligned} \tag{3.1.7}$$

The involution is the adjoint operation with respect to the standard scalar product in the tensor product of $\mathbb{C}^n$. For low-temperature expansions of (3.1.2) it is more convenient to consider a representation $\tilde{r}$ different from r:

$$\begin{aligned} \tilde{r}(\Gamma_j)\,|\, i_1 \ldots i_j \ldots i_N \rangle &= \omega^{i_j} \,|\, i_1 \ldots i_j \ldots i_N \rangle \\ \tilde{r}(\sigma_j)\,|\, i_1 \ldots i_j \ldots i_N \rangle &= |\, i_1 \ldots (i_j - 1 \bmod n) \ldots i_N \rangle \,. \end{aligned} \tag{3.1.8}$$

The Hamiltonian (3.1.1) commutes with the $\mathbb{Z}_n$ charge operator $\hat{Q} := \prod_{j=1}^N \sigma_j$ acting on the vectors (3.1.6) as

$$r(\hat{Q})\,|\, i_1 \ldots i_N \rangle = \omega^{\left(\sum_{j=1}^N i_j\right)} \,|\, i_1 \ldots i_N \rangle \tag{3.1.9}$$

which shows that the eigenvalues of $\hat{Q}$ have the form ω^Q with Q integer. Thus, $H_N^{(n)}$ has n charge sectors which we shall refer to by $Q = 0, \ldots, n-1$.

$H_N^{(n)}$ also commutes with the translation operator T_N that acts on the basis vectors (3.1.6) in the following way:

$$r(T_N)\mid i_1 i_2 \dots i_N\rangle \;=\mid i_2 \dots i_N i_1\rangle\,. \tag{3.1.10}$$

The eigenvalues of T_N are Nth roots of unity. We label them by e^{iP} and call P the 'momentum'. We choose $0 \le P < 2\pi$ corresponding to the first Brillouin zone and have $P \in \{0, \frac{2\pi}{N}, \dots, \frac{2\pi(N-1)}{N}\}$. Note that the states

$$\begin{aligned}\| i_1 i_2 \dots i_{N-1} i_N\rangle\rangle_P := \frac{1}{\sqrt{\mathcal{N}}}\Big(&\mid i_1 i_2 \dots i_{N-1} i_N\rangle + e^{iP}\mid i_N i_1 i_2 \dots i_{N-1}\rangle + \dots \\ &+ e^{iP(N-1)}\mid i_2 \dots i_{N-1} i_N i_1\rangle\Big)\end{aligned} \tag{3.1.11}$$

are eigenstates of T_N with eigenvalue e^{iP}. $\mathcal{N}$ is a suitable normalization constant. If the state $\mid i_1 \dots i_N\rangle$ has no symmetry (i.e. $T_N^k \mid i_1 \dots i_N\rangle \;\neq\mid i_1 \dots i_N\rangle$ for all $0 < k < N$), one has $\mathcal{N} = N$. This will apply to most cases below where we need (3.1.11). For a definition of the momentum eigenstates (3.1.11) in case of cyclic boundary conditions $R \neq 0$ see e.g. [73, 40]

We will frequently use the following parameterization of the constants α_k and $\bar{\alpha}_k$, fixing their dependence on k:

$$\alpha_k = \frac{e^{i\phi(\frac{2k}{n}-1)}}{\sin\frac{\pi k}{n}}\,, \qquad \bar{\alpha}_k = \frac{e^{i\varphi(\frac{2k}{n}-1)}}{\sin\frac{\pi k}{n}}. \tag{3.1.12}$$

This is a suitable choice because it includes a large class of interesting models.

For $\phi = \varphi = 0$ one obtains real $\alpha_k = \bar{\alpha}_k = \frac{1}{\sin\frac{\pi k}{n}}$. This leads to models with a second order phase transition at $\lambda = 1$ which can be described by a parafermionic conformal field theory in the limit $N \to \infty$ at criticality [56, 8]. These so-called Fateev-Zamolodchikov-models [57] lead to extended conformal algebras $\mathcal{WA}_{n-1}$ where the simple fields have conformal dimension $2, \dots, n$ [54]. The spectrum of the Hamiltonian (3.1.1) can be described by the first unitary minimal model of the algebra $\mathcal{WA}_{n-1}$. For $n = 3$ the symmetry algebra is Zamolodchikov's well-known spin-three extended conformal algebra [129] at $c = \frac{4}{5}$.

Choosing $\phi = \varphi = \frac{\pi}{2}$ in (3.1.12) for the Hamiltonian (3.1.1) one recovers the superintegrable $\mathbb{Z}_n$-chiral Potts model (2.4.8).

The parameterization (3.1.12) also includes the family of integrable models discovered in refs. [4, 5, 6, 10, 11, 12] which interpolates between the integrable cases at $\phi = \varphi = 0$, $\lambda = 1$ and $\phi = \varphi = \frac{\pi}{2}$. The Hamiltonian (3.1.1) is integrable if one imposes the additional constraint

$$\cos\varphi = \lambda\cos\phi \tag{3.1.13}$$

(or equivalently $\tilde{\lambda}\cos\varphi = \cos\phi$ for the low-temperature phase) on the parameterization (3.1.12). For $\phi = \varphi = 0$ this yields $\lambda = 1$ – the conformally invariant critical points. At

$\phi = \varphi = 0$, the Hamiltonian is self-dual, i.e. it is invariant under a duality-transformation such that $H_N^{(n)}(\lambda) \cong \lambda H_N^{(n)}(\lambda^{-1})$. The Hamiltonian is also self-dual on the superintegrable line $\phi = \varphi = \frac{\pi}{2}$. $H_N^{(n)}$ with the choices (3.1.12), (3.1.13) is in general not self-dual any more whereas particular choices yield a self-dual Hamiltonian. If we choose for (3.1.12) $\phi = \varphi$ and neglect (3.1.13) $H_N^{(n)}$ will be self-dual again. Therefore we choose to refer to (3.1.1) with (3.1.12) as the general 'chiral Potts model'. We will not consider the integrable case where the additional constraint (3.1.13) is satisfied in detail.

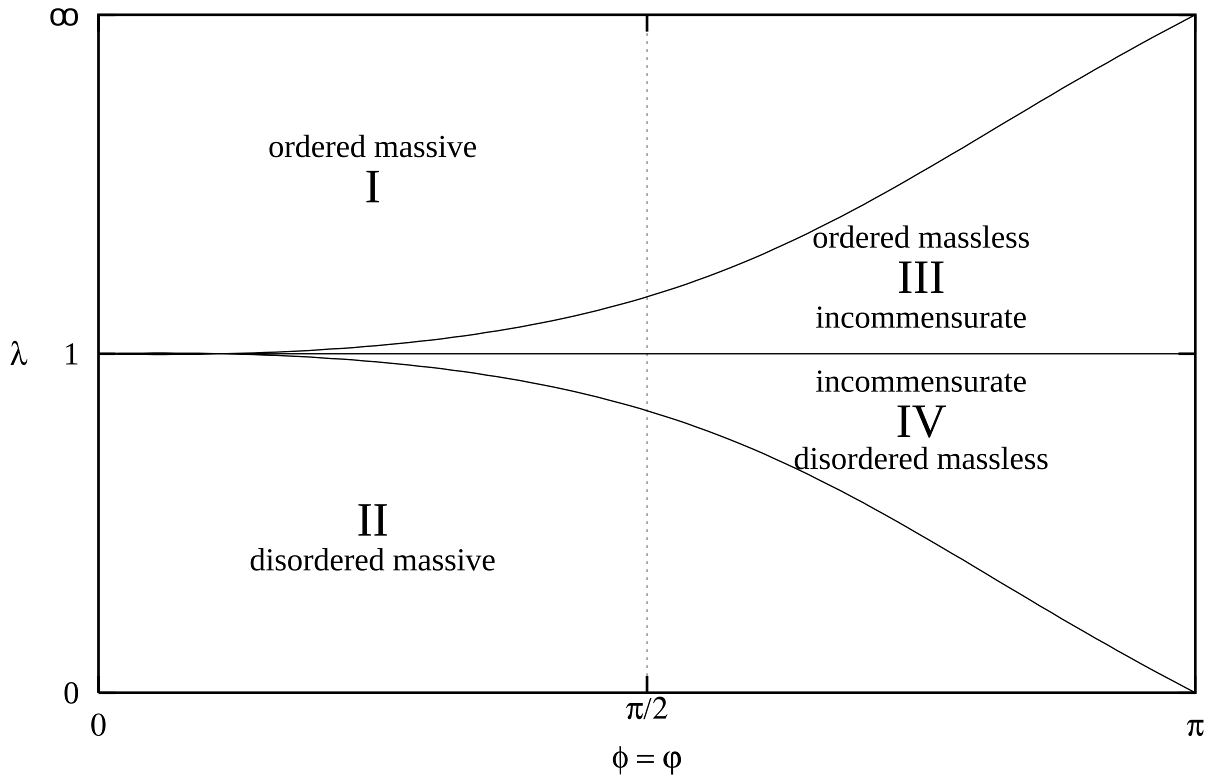

Fig. 1: Schematic phase diagram of the self-dual chiral Potts model for $n = 3$.

The main features of the phase diagram of the $\mathbb{Z}_n$-chiral Potts chain are already present for $n = 3$. The $\mathbb{Z}_3$ version of (3.1.1) is known to have four phases [4, 6, 66]: Two massive and two massless phases (see Fig. 1). One of the massive phases is ordered and the other massive phase is disordered. In the following we will mainly be interested in the massive phases. At $\phi = \varphi = \frac{\pi}{2}$ the massive high-temperature phase (small λ) appears in the range $0 \leq \lambda \leq 0.901292\ldots$ and the massive low-temperature phase appears in the range $1/0.901292\ldots \leq \lambda \leq \infty$ [4, 6]. There is a second order phase transition at the point $\lambda = 1$ for $\phi = \varphi = 0$ and general $\mathbb{Z}_n$. This conformally invariant point is described by the models of Fateev and Zamolodchikov with $\mathcal{WA}_{n-1}$-symmetry [56, 57, 8, 54]. The conformal field theories can be perturbed by a thermal operator (see e.g. [58, 130, 131, 132, 111]). This perturbation is integrable and corresponds to going to $\lambda \neq 1$ on the line $\phi = \varphi = 0$ of the $\mathbb{Z}_n$-quantum spin chain. One can also introduce an integrable chiral perturbation of the conformal field theories [38]. The $\mathbb{Z}_n$-spin quantum chains describe both this chiral perturbation as well as the integrable thermal perturbations.

Our main interest is the spectrum in the limit $N \to \infty$ of $H_N^{(n)}$. Of course, we have to specify how the limit is to be taken. One possible definition was given in [91]. Here, we want to omit the technical details. We just mention that the basic idea is first to identify momentum eigenstates for chains of different lengths and then to consider the weak limit of T_N and the excitation spectrum operator

$$\Delta H_N^{(n)} := H_N^{(n)} - E_N^0 \mathbb{1} \tag{3.1.14}$$

where E_N^0 is the groundstate energy for N sites.

3.2. Duality of spectra

There is a first statement about the spectra of the Hamiltonian (3.1.1) which allows us to restrict to the high-temperature phase $\lambda < 1$ for the discussion of the spectrum: The spectra in the high-temperature phase at λ are *dual* to those in the low-temperature phase at $\lambda = \tilde{\lambda}$ if we interchange α_k and $\bar{\alpha}_k$. This statement for $\mathbb{Z}_n$-quantum spin chains has been known for a long time [52, 92] and was also used in [97]. However, special attention has to be paid to the boundary conditions when performing duality transformations. It has been observed in [70] that the duality transformation interchanges the rôle of the charge Q and boundary conditions R. The precise statement is given by the following

Theorem V: *(Duality) Denote the Hamiltonian (3.1.1) by $H_N^{(n)}(\lambda, R^{ht}, \bar{\alpha}_k^{ht}, \alpha_k^{ht})$ and (3.1.2) by $\tilde{H}_N^{(n)}(\tilde{\lambda}, R^{lt}, \bar{\alpha}_k^{lt}, \alpha_k^{lt})$, including in both cases explicitly the corresponding parameters. Furthermore, abbreviate the space with charge Q^{ht} in the high-temperature phase by $\mathcal{H}^{Q^{ht}}$ and the eigenspace of $\tilde{r}(\hat{Q})$ to eigenvalue $\omega^{Q^{lt}}$ by $\tilde{\mathcal{H}}^{Q^{lt}}$. Then $H_N^{(n)}(\lambda, R^{ht}, \bar{\alpha}_k^{ht}, \alpha_k^{ht})$ restricted to $\mathcal{H}^{Q^{ht}}$ and $\tilde{H}_N^{(n)}(\tilde{\lambda}, R^{lt}, \bar{\alpha}_k^{lt}, \alpha_k^{lt})$ restricted to $\tilde{\mathcal{H}}^{Q^{lt}}$ have the same spectra if*

$$\begin{aligned} Q^{lt} &= R^{ht} \,, \qquad R^{lt} = Q^{ht} \,, \\ \bar{\alpha}_k^{lt} &= \alpha_k^{ht} \,, \qquad \alpha_k^{lt} = \bar{\alpha}_k^{ht} \,, \qquad \tilde{\lambda} = \lambda . \end{aligned} \tag{3.2.1}$$

■

Proof: We present a simple non-standard proof of theorem V [82] that is different from the approach of e.g. [52, 92]. We derive duality by comparing the representation r (3.1.7) to the representation $\tilde{r}$ (3.1.8). Working with the states has the advantage that it is straightforward to take care of the boundary conditions. Note that $\tilde{r}(\Gamma_j) = r(\sigma_j)$ and $\tilde{r}(\sigma_j) = r(\Gamma_j^+)$ and that the representations $\tilde{r}$ and r are unitarily equivalent. Now fix the state $|\,\mathrm{GS}\rangle^{\,Q^{lt}}$ to be the ground state in $\tilde{\mathcal{H}}^{Q^{lt}}$:

$$|\,\mathrm{GS}\rangle^{\,Q} := \frac{1}{\sqrt{n}} \sum_{l=0}^{n-1} \omega^{l \cdot Q} \,|\, l \ldots l\rangle \,. \tag{3.2.2}$$

Then the following states are a basis for $\tilde{\mathcal{H}}^{Q^{lt}}$:

$$|\, Q; i_2 \ldots i_N\rangle := \tilde{r}(\sigma_2^{-i_2}) \ldots \tilde{r}(\sigma_N^{-i_N}) \,|\,\mathrm{GS}\rangle^{\,Q^{lt}} . \tag{3.2.3}$$

Note that this implies:

$$\tilde{r}(\sigma_1)\,|Q; i_2 \dots i_N\rangle \;= \omega^{Q^{lt}}\;|Q; (i_2+1)\dots(i_N+1)\rangle\,. \tag{3.2.4}$$

Now consider the following intertwining isomorphism I:

$$I\,|Q; i_2 \dots i_N\rangle \;:=|(-i_2)(i_2-i_3)\dots(i_{N-1}-i_N)(i_N+R^{lt})\rangle\,. \tag{3.2.5}$$

It is now straightforward to check using the basis (3.2.3) that

$$I\tilde{r}(\sigma_{(j+1 \bmod N)}) = r(\Gamma_j\Gamma_{j+1}^{+})I\;, \qquad I\tilde{r}(\Gamma_j\Gamma_{j+1}^{+}) = r(\sigma_j)I\;. \tag{3.2.6}$$

The observation that I is a unitary map and r and $\tilde{r}$ are unitarily equivalent in conjunction with (3.2.6) concludes the proof. $\square$

Remarks:

1) The momentum decomposition can be applied alike in the high- and low-temperature phase. Thus, theorem V is also valid if we further restrict to eigenspaces with momentum P.
2) Duality (3.2.1) preserves the condition (3.1.13). Thus, each integrable chiral Potts model is dual to exactly one integrable chiral Potts model.

3.3. Generalities about perturbation theory

Some of the results that will be reported later on rely on perturbation theory. Therefore, we now review the general outline for perturbation theory to all orders as presented in [23] which directly applies to the degenerate case as well. It should be clear to the reader that this method is not in all cases the most powerful one available. Nevertheless, unlike e.g. cluster expansions it can be directly applied to any problem we are interested in (including higher excitations and correlation functions). Note also that we do not intend to study the massless regimes III and IV of Fig. 1 for which perturbation expansions are certainly not well suited.

The Hamiltonian (3.1.1) can be written as $H = H_0 + \lambda V$ with $H_0 = -\sum_{j,k}\bar{\alpha}_k\sigma_j^k$, $V = -\sum_{j,k}\alpha_k\Gamma_j^k\Gamma_{j+1}^{n-k}$. The eigenstates for H_0 are obvious, thus we have solved:

$$H_0\;|a\rangle\;= E^{(0)}_{|a\rangle}\;|a\rangle\,. \tag{3.3.1}$$

Now one can solve $H\;|\,a(\lambda)\rangle \;=\; E_{|a\rangle}\;\;|\,a(\lambda)\rangle$ for small λ as follows: Let $q_{|a\rangle}$ be the projector onto the eigenspace of H_0 with eigenvalue $E^{(0)}_{|a\rangle}$. We can treat non-degenerate and degenerate perturbation theory alike if we choose $|\,a\rangle$ such that

$$q_{|a\rangle}\,V\;|\,a\rangle\;= E^{(1)}_{|a\rangle}\;|\,a\rangle \tag{3.3.2}$$

with a constant $E^{(1)}_{|a\rangle}$, i.e. $q_{|a\rangle}\,Vq_{|a\rangle}$ is to be chosen diagonal. One also needs a regularized resolvent $g(z)$ of H_0:

$$g(z) := \left(\mathbb{1} - q_{|a\rangle}\right)(z - H_0)^{-1}\,. \tag{3.3.3}$$

Then, the Wigner-Brillouin perturbation series

$$E_{|a\rangle} = \sum_{\nu=0}^{\infty} \lambda^\nu E_{|a\rangle}^{(\nu)} \, , \qquad |\, a(\lambda)\rangle = \sum_{\nu=0}^{\infty} \lambda^\nu \; |\, a, \nu\rangle \tag{3.3.4}$$

are given by the following recurrence relations [23]:

$$\begin{aligned} |\, a, 0\rangle \; &= |\, a\rangle \\ |\, a, \nu\rangle \; &= g(E_{|a\rangle}^{(0)}) \left\{ V \; |\, a, \nu - 1\rangle \; - \sum_{\mu=1}^{\nu-1} |\, a, \nu - \mu\rangle \; E_{|a\rangle}^{(\mu)} \right\} , \\ E_{|a\rangle}^{(\nu+1)} &= \langle a \,| \;\; V \; |\, a, \nu\rangle \, . \end{aligned} \tag{3.3.5}$$

Note that neither $|\, a(\lambda)\rangle$ nor $|\, a, \nu\rangle$ are in general normalized although $|\, a\rangle$ must be normalized to one. Observe that the derivation of (3.3.5) does not rely on H being hermitean. Therefore, (3.3.5) may also be applied to diagonalizable but non-hermitean H.

The radius of convergence of the series (3.3.4) can be more easily discussed in a different framework. Therefore, we postpone such a discussion to section 4.5.

There is one observation that makes explicit evaluation of high orders for the $\mathbb{Z}_n$-Hamiltonian (3.1.1) possible. The energy-eigenvalues $E_{|a\rangle}$ of $H_N^{(n)}$ do depend on the chain length N. However, for the low lying gaps $\Delta E_{|a\rangle}$ [2]) of $\Delta H_N^{(n)}$ (see (3.1.14)) the coefficients for powers of λ become independent of N up to order λ^{N-2} (see e.g. [7]). Intuitively, this can be inferred from the fact that (3.1.1) shows only nearest neighbour interaction and thus we need $N - 1$ powers in V to bring us around a chain of length N. Smaller powers in V (or λ) do not feel that the length of the chain is finite.

[2]) This will apply precisely to the fundamental quasiparticle states to be discussed below.

Paa den anden Side møder vi Vanskeligheder af en saa dybtliggende Natur, at vi ikke aner Vejen til deres Løsning; efter min personlige Opfattelse er disse Vanskeligheder af en saadan Art, at de næppe lader os haabe indenfor Atomernes Verden at gennemføre en Beskrivelse i Rum og Tid af den Art, der svarer til vore Saedvanlige Sansebilleder.

Niels Bohr, Letter to Høffding in 1922

4. Excitation spectrum

In this chapter we will study the excitation spectrum of the $\mathbb{Z}_n$-chiral Potts model. For this end we denote the kth gap in charge sector Q by $\Delta E_{Q,k}$ starting to count with $k = 0$. More precisely, we define

$$\Delta E_{Q,k}(P) := E_{Q,k}(P) - E_{0,0}(0) \tag{4.1}$$

where $E_{Q,k}(P)$ is the kth energy level with momentum P in charge sector Q. In the massive phases the groundstate has $Q = P = 0$, i.e. $E_{0,0}(0)$ is the energy of the groundstate. We will mainly be interested in the thermodynamic limit, i.e. in the limit $N \to \infty$ of (4.1). Thus, if we write down energy gaps $\Delta E_{Q,k}(P)$ we will usually think of sufficiently large lattices. It will be clear from the context when gaps are evaluated for particular finite chain length N.

In general we have the following symmetry under charge conjugation

$$\Delta E_{n-Q,k}(P,\phi,\varphi) = \Delta E_{Q,k}(P,-\phi,-\varphi). \tag{4.2}$$

Therefore, it is sufficient to restrict to those charge sectors with $Q \leq \frac{n}{2}$ in all explicit calculations where we keep the dependence on ϕ and φ.

4.1. Analytic results for the superintegrable $\mathbb{Z}_3$-chain

The results in [41, 103] and [68, 69, 91] suggest that we may expect a quasiparticle spectrum in the complete massive high-temperature phase of the general $\mathbb{Z}_n$-Hamiltonian (3.1.1). At $\phi = \varphi = \frac{\pi}{2}$ the spectrum of the Hamiltonian (3.1.1) has been determined analytically by McCoy et al. [41] for $n = 3$. Their result is that the spectrum is a perfect quasiparticle spectrum. We formulate their precise result in this section.

Def. IV: ([41]) Let

$$\begin{aligned} \mathsf{E}_1(P_r) = e_r &= 2 \mid 1-\lambda \mid + \frac{3}{\pi}\int_1^{\left|\frac{1+\lambda}{1-\lambda}\right|^{\frac{2}{3}}} \mathrm{d}t \frac{v_r(2v_r t+1)}{v_r^2 t^2 + v_r t + 1}\sqrt{\frac{4\lambda}{t^3-1} - (1-\lambda)^2}\,, \\ \mathsf{E}_2(P_{2s}) = e_{2s} &= 4 \mid 1-\lambda \mid + \frac{3}{\pi}\int_1^{\left|\frac{1+\lambda}{1-\lambda}\right|^{\frac{2}{3}}} \mathrm{d}t \frac{v_{2s}(4v_{2s}^2 t^2 - v_{2s} t + 1)}{v_{2s}^3 t^3 + 1}\sqrt{\frac{4\lambda}{t^3-1} - (1-\lambda)^2} \end{aligned} \tag{4.1.1}$$

with the auxiliary variables v_r and v_{2s} related to the momenta by:

$$
\begin{aligned}
v_r &= \frac{e^{iP_r}-1}{\omega(\omega e^{iP_r}-1)}\,, \qquad & 0 \le P_r < 2\pi\,, \\
v_{2s} &= \frac{e^{iP_{2s}}-1}{e^{-i\frac{\pi}{3}}e^{iP_{2s}}-e^{i\frac{\pi}{3}}}\,, \qquad & \frac{2\pi}{3} \le P_{2s} \le 2\pi\,.
\end{aligned}
\tag{4.1.2}
$$

Note that the Brillouin zone of the $Q=2$ excitation is only the interval $[\frac{2\pi}{3}, 2\pi]$.

It is very difficult to evaluate the integrals in (4.1.1) explicitly except for a few special values of the momentum. One can check that

$$P_r = 0 \quad \Rightarrow \quad v_r = 0 \quad \Rightarrow \quad e_r = 2|1-\lambda|\,, \tag{4.1.3a}$$
$$P_{2s} = 0 \quad \Rightarrow \quad v_{2s} = 0 \quad \Rightarrow \quad e_{2s} = 4|1-\lambda|\,, \tag{4.1.3b}$$
$$P_r \to \tfrac{4\pi}{3} \quad \Rightarrow \quad v_r \to \pm\infty \quad \Rightarrow \quad e_r = 2(1+\lambda)\,, \tag{4.1.3c}$$
$$P_{2s} \to \tfrac{2\pi}{3} \quad \Rightarrow \quad v_{2s} \to \infty \quad \Rightarrow \quad e_{2s} = 4(1+\lambda)\,. \tag{4.1.3d}$$

This shows that even for infinite values of the rapidities the energy as a function of the physical variable momentum P is well-defined. Thus, as a function of P the $Q=1$ excitation has *no* singularity at $P = \frac{4\pi}{3}$ and also e_{2s} is continuous at both boundaries including $P = \frac{2\pi}{3}$. For other values of the momentum than in (4.1.3) one can perform numerical integration where special attention has to be paid to the singularities in the integrand at $t=1$.

Proposition I: *([41]) All excitations above the groundstate can be composed in the large chain limit of the fundamental excitations $\mathsf{E}_1(P) := e_r(P)$ and $\mathsf{E}_2(P) := e_{2s}(P)$ according to the following rules:*

$$\Delta E_{Q,r}(P,\phi,\varphi) = \sum_{k=1}^{m_r} \mathsf{E}_{Q^{(k)}}(P^{(k)})\,, \quad P = \sum_{k=1}^{m_r} P^{(k)} \ mod\ 2\pi\,, \quad Q = \sum_{k=1}^{m_r} Q^{(k)} \ mod\ n. \tag{4.1.4}$$

subject to the Pauli principle, i.e. $Q^{(i)} = Q^{(j)}$ implies $P^{(i)} \ne P^{(j)}$. ■

It was argued in [103] by examining the zeroes of the transfer matrix that the same statement should also apply to the integrable three states chain although here the relation between rapidities and momentum is not known.

For a detailed comparison with numerical methods and the perturbative approach to be presented below see [69].

4.2. High-temperature expansions

In order to generalize the quasiparticle picture of the previous section we first study the low lying levels in the spectrum of the chiral Potts model perturbatively in this section. In particular, for $n=3$ and $n=4$ we calculate the dispersion relations of the lowest excitations in the charge sectors $Q \ne 0$. Some first results in this direction have been presented in [68] for the self-dual version of these models. In this section we derive higher orders and admit general $\phi \neq \varphi$. We also present some explicit results on the next excitations.

In [97] high-temperature perturbation series were computed for the disorder operator (or magnetization m) and the first energy gap in the momentum zero sector of the superintegrable $\mathbb{Z}_3$-chiral Potts model leading to exact conjectures for both of them. After the superintegrable chiral Potts model had been generalized to general n [70] perturbation series for the ground state energy, energy gap in the momentum zero sector, magnetization and susceptibility of this superintegrable $\mathbb{Z}_n$-chiral Potts model were presented in [83]. At the same time elaborate expansions of the ground state energy and some excitations of the superintegrable chiral Potts model for $n \in \{3, 4, 5\}$ and in particular perturbation series for the order parameters with general n were calculated in [7]. First perturbative results for the energy gaps at more general values of the angles ϕ, φ were obtained in [68] where second order high-temperature expansions for the translationally invariant energy gaps in each charge sector of the general self-dual $\mathbb{Z}_3$- and $\mathbb{Z}_4$-chiral Potts models as well as a first order expansion for the dispersion relations for general n was presented.

For arbitrary n, N the groundstate of the Hamiltonian (3.1.1) in the limit $\lambda \to 0$ is given by:

$$|\,\mathrm{GS}\rangle :=|\,0\ldots0\rangle \tag{4.2.1}$$

provided that $-\frac{\pi}{2} \leq \varphi \leq \frac{\pi}{2}$. For $n = 3$ (4.2.1) will be the groundstate for the larger range $-\pi \leq \varphi \leq \pi$ and for $n = 4$ (4.2.1) is the groundstate for $-\frac{5\pi}{6} \leq \varphi \leq \frac{5\pi}{6}$.

The first excited states at $\lambda = 0$ for $Q > 0$ and arbitrary P are the states

$$\|s^Q\rangle\rangle_{\,P} := \|Q0\ldots0\rangle\rangle_{\,P} \tag{4.2.2}$$

in the range $-\frac{\pi}{2} \leq \varphi \leq \frac{\pi}{2}$. According to the definition of the Hilbert space $\mathcal{H}$ in [91], the states (4.2.2) give rise to proper eigenstates in the limit of $\Delta H^{(n)}$. Thus, the corresponding gaps $\Delta E_{Q,0}(P)$ belong to the point spectrum of $\Delta H^{(n)}$.

More generally, we wish to argue later on that the complete spectrum can be explained in terms of quasiparticles. At $\lambda = 0$, a single-particle excitation corresponds to just one flipped spin (4.2.2). Due to the absence of interactions k-particle states have k flipped spins at $\lambda = 0$. Therefore, one can think in terms of states keeping in mind that for $\lambda > 0$ one has to take the interactions into account using perturbation theory. Note, however, that except for the single-particle states and certain two-particle states we cannot directly compute the perturbation series for multi-particle states and check that they have the correct properties. Nevertheless, such a picture may be suggestive and is in fact traditional (see e.g. [35] for a transfer-matrix approach to the spectrum of the Ising model in d dimensions).

First, one can derive a first order expansion for the dispersion relations of the lowest excitations in the charge sectors $0 < Q < n$ using (4.2.1) and (4.2.2) [68]:

$$\Delta E_{Q,0}(P, \bar{\alpha}_k, \phi) = \left(\sum_{k=1}^{n} \bar{\alpha}_k \left(1 - \omega^{Q\,k}\right)\right) - \frac{2\lambda}{\sin\left(\frac{\pi Q}{n}\right)} \cos\left(P - \left(1 - \frac{2Q}{n}\right)\phi\right) + \mathcal{O}(\lambda^2). \tag{4.2.3}$$

From (4.2.3) we can immediately read off that in the limit $\lambda \to 0$ the minimum of the dispersion relations $P_{\min,Q}$ is located at

$$P_{\min,Q} = \left(1 - \frac{2Q}{n}\right)\phi \tag{4.2.4}$$

which demonstrates that for $\phi \neq 0$ parity is not conserved.

Let us now specialize to the $\mathbb{Z}_3$-chain. We will use the abbreviations:

$$\begin{gathered}\mathcal{C} := \cos\left(\frac{\varphi}{3}\right), \qquad \widehat{\mathcal{C}} := \cos\left(\frac{\pi-\varphi}{3}\right), \qquad \mathcal{R} := 1 - 4\mathcal{C}^2 , \qquad \mathcal{U} := 7\mathcal{R} - 4 , \\ \bar{\mathcal{C}}_r : = \cos\left(\frac{r\phi}{3}\right).\end{gathered} \tag{4.2.5}$$

For $n = 3$ we can calculate the groundstate energy per site e_0 which is defined by $E_N^0 = N e_0$ perturbatively:

$$\begin{aligned} e_0 = & -\frac{4}{\sqrt{3}}\mathcal{C} - \frac{2\lambda^2}{3\sqrt{3}\mathcal{C}} - \frac{\cos(\phi)\lambda^3}{9\sqrt{3}\mathcal{C}^2} + \frac{\sqrt{3}}{81\mathcal{C}}\left\{\frac{1}{2\mathcal{C}^2} + \frac{4}{\mathcal{R}}\right\}\lambda^4 + \frac{\sqrt{3}\cos(\phi)}{81\mathcal{C}^2}\left\{\frac{3}{4\mathcal{C}^2} + \frac{4}{\mathcal{R}}\right\}\lambda^5 \\ & + \frac{1}{\sqrt{3}}\left[\frac{\cos(2\phi)}{324\mathcal{C}^3}\left\{\frac{6}{\mathcal{R}} + \frac{1}{\mathcal{C}^2}\right\} + \frac{23}{3888\mathcal{C}^5}\right. \\ & \qquad \left. + \frac{1}{9\mathcal{U}}\left\{-\frac{40}{81\mathcal{C}\mathcal{R}} + \frac{8}{\mathcal{C}\mathcal{R}^2} - \frac{32}{27\mathcal{C}\mathcal{R}^3} - \frac{11}{27\mathcal{C}^3\mathcal{R}} - \frac{28}{27\mathcal{C}^3\mathcal{R}^2} + \frac{55}{27\mathcal{C}^3}\right\}\right]\lambda^6 \\ & + \frac{\cos(\phi)}{\sqrt{3}}\left[-\frac{1}{324\mathcal{C}^6} + \frac{1}{729\mathcal{U}^2}\left\{\frac{63976}{9\mathcal{C}^2\mathcal{R}} - \frac{47972}{9\mathcal{C}^2\mathcal{R}^2} + \frac{3104}{3\mathcal{C}^2\mathcal{R}^3} - \frac{64}{\mathcal{C}^2\mathcal{R}^4} + \frac{6664}{9\mathcal{C}^2}\right.\right. \\ & \qquad \left.\left. - \frac{2326}{3\mathcal{C}^4\mathcal{R}} + \frac{284}{\mathcal{C}^4\mathcal{R}^2} + \frac{3529}{12\mathcal{C}^4}\right\}\right]\lambda^7 + \mathcal{O}(\lambda^8). \end{aligned} \tag{4.2.6}$$

For $\varphi = \phi = \frac{\pi}{2}$ (4.2.6) reproduces the result of [83]. The orders $e_0^{(k)}$ of the free energy per site e_0 are independent of N if $N > k$. Comments on the accuracy of a truncation to 5th order of (4.2.6) can be found in [82, 91].

In principle, one can derive a critical exponent α for the specific heat $\frac{\mathrm{d}^2 e_0}{\mathrm{d}\lambda^2}$ from a perturbation expansion of the ground state energy e_0. In fact, α has been estimated using a 13th order expansion of e_0 in [97] for the self-dual case $\phi = \varphi$ and for the superintegrable case $\phi = \varphi = \frac{\pi}{2}$ the Ising-like form of the eigenvalues has been exploited to calculate even higher orders of e_0 in [7]. The results in [97, 7] indicate $\alpha = \frac{1}{3}$ independent of the angles ϕ, φ.

We omit the results presented for the lowest translationally invariant gaps of the three states chain presented in [91]. For $n = 3$ and general P we obtain from the states (4.2.2) the perturbation expansion (4.2.7) below for the dispersion relation of the lowest $Q = 1$ excitation and the lowest $Q = 2$ excitation is given by (4.2) [3]). In [69, 91] we restricted

[3]) The fourth order was independently obtained by G. von Gehlen using the slightly more compact notation of [69].

to a 3rd order version of (4.2.7) because of the complicatedness of the 4th order which we present here just as an illustration. It is also not difficult to compute the 5th order on a computer but we do not want to present this to the reader here either.

$$
\begin{aligned}
\mathsf{E}_1(P) := \Delta E_{1,0}(P,\phi,\varphi) &= 4\sin\left(\frac{\pi-\varphi}{3}\right) - \lambda\frac{4}{\sqrt{3}}\cos\left(P-\frac{\phi}{3}\right) \\
&- \lambda^2\frac{2}{3\sqrt{3}}\left\{\frac{\cos\left(P+\frac{2\phi}{3}\right)+1}{\widehat{\mathcal{C}}} + \frac{\cos\left(2P-\frac{2\phi}{3}\right)-2}{\mathcal{C}}\right\} \\
&+ \lambda^3\frac{1}{9\sqrt{3}}\left\{-\frac{2\cos\left(2P+\frac{\phi}{3}\right)-3\cos\left(P-\frac{\phi}{3}\right)+2\cos(3P-\phi)-2\cos(\phi)}{\mathcal{C}^2}\right. \\
&\left. - \frac{2\cos\left(2P+\frac{\phi}{3}\right)+2\cos\left(P-\frac{\phi}{3}\right)}{\mathcal{C}\widehat{\mathcal{C}}} + \frac{\cos\left(2P+\frac{\phi}{3}\right)+2\cos\left(P-\frac{\phi}{3}\right)+\cos(\phi)}{\widehat{\mathcal{C}}^2}\right\} \\
&+ \lambda^4\left[\frac{1}{54\sqrt{3}}\left\{\left(\frac{6}{\mathcal{C}^3}+\frac{4}{\mathcal{C}\widehat{\mathcal{C}}^2}-\frac{2}{\widehat{\mathcal{C}}^3}\right)\cos\left(2P-\frac{2\phi}{3}\right) - \left(\frac{4}{\mathcal{C}^3}-\frac{3}{\mathcal{C}\widehat{\mathcal{C}}^2}+\frac{1}{\widehat{\mathcal{C}}^3}\right)\cos(3P)\right.\right. \\
&\quad - \left(\frac{1}{\mathcal{C}^3}+\frac{2}{\mathcal{C}\widehat{\mathcal{C}}^2}+\frac{1}{\mathcal{C}^2\widehat{\mathcal{C}}}\right)\cos\left(2P+\frac{4\phi}{3}\right) \\
&\quad + \left(\frac{2}{\mathcal{C}^3}+\frac{1}{\mathcal{C}\widehat{\mathcal{C}}^2}-\frac{1}{\widehat{\mathcal{C}}^3}-\frac{1}{\mathcal{C}^2\widehat{\mathcal{C}}}\right)\cos\left(P-\frac{4\phi}{3}\right) - \frac{5}{\mathcal{C}^3}\cos\left(4P-\frac{4\phi}{3}\right) \\
&\quad \left. + \left(\frac{6}{\mathcal{C}^3}+\frac{16}{\mathcal{C}\widehat{\mathcal{C}}^2}-\frac{2}{\widehat{\mathcal{C}}^3}+\frac{20}{\mathcal{C}^2\widehat{\mathcal{C}}}\right)\cos\left(P+\frac{2\phi}{3}\right) - \frac{5}{\mathcal{C}^3}+\frac{18}{\mathcal{C}\widehat{\mathcal{C}}^2}-\frac{2}{\widehat{\mathcal{C}}^3}+\frac{18}{\mathcal{C}^2\widehat{\mathcal{C}}}\right\} \\
&\quad - \frac{1}{9\sin\left(\frac{\pi+\varphi}{3}\right)}\left\{\left(\frac{1}{\mathcal{C}^2}+\frac{2}{\mathcal{C}\widehat{\mathcal{C}}}+\frac{1}{\widehat{\mathcal{C}}^2}\right)\cos\left(P+\frac{2\phi}{3}\right)+\frac{2}{3\mathcal{C}^2}+\frac{2}{\mathcal{C}\widehat{\mathcal{C}}}+\frac{1}{\widehat{\mathcal{C}}^2}\right. \\
&\quad \left.\left. +\frac{2}{9}\left(\frac{1}{\mathcal{C}^2}+\frac{1}{\mathcal{C}\widehat{\mathcal{C}}}\right)\left(\cos\left(2P-\frac{2\phi}{3}\right)+\cos(3P)\right)\right\} - \frac{2\cos(3P)-3}{81\sin\left(\frac{\pi-\varphi}{3}\right)\mathcal{C}^2}\right] + \mathcal{O}(\lambda^5)\,.
\end{aligned}
\tag{4.2.7}
$$

Note that the agreement even of the truncations to 3rd order of (4.2.7) with the results of a numerical diagonalization is usually good as was discussed in detail in [69] and in [91] for $\phi = \varphi = P = 0$.

We would like to mention that after specializing (4.2.7) to $\phi = \varphi = 0$ it becomes much simpler and it even makes sense to also present the 5th order [91]. For $\phi = \varphi = 0$ one can read off from (4.2.7) that for λ small, a Klein-Gordon dispersion relation is a good approximation. It was shown in [2] that for $\phi = \varphi = 0$ and in the limit $\lambda = 1$ one obtains $\mathcal{E}_1(P) = 6|\sin\left(\frac{P}{2}\right)|$ which is also of the Klein-Gordon form on the lattice. However, one can show that for general λ and $\phi = \varphi = 0$ a Klein-Gordon relation is nothing but a very good approximation to $\mathsf{E}_1(P)$ [91]. Also certain generalizations of Klein-Gordon dispersion relations can be ruled out [91].

In section 3.3 we mentioned that the kth orders of (4.2.5) – (4.2.7) are independent of N if $N \geq k+2$. In particular, this implies the existence of the limits $N \to \infty$ of (4.2.6) and

(4.2.7) if the perturbation series converge at all.

In the derivation of (4.2.7) we have not assumed that the Hamiltonian (3.1.1) is hermitean. Thus, we may admit $\phi \in \mathbb{C}$. We have checked in a few cases that results of a numerical diagonalization at $N = 12$ sites are still in good agreement with (4.2.7) also for complex ϕ.

For the $\mathbb{Z}_4$-chain one obtains up to second order in λ:

$$
\begin{aligned}
\Delta E_{1,0}(P,\phi,\varphi) &= 2\left(1 + 2\sin\left(\frac{\pi - 2\varphi}{4}\right)\right) - \lambda 2\sqrt{2}\cos\left(P - \frac{\phi}{2}\right) \\
&- \lambda^2 \left\{ \frac{2\sqrt{2}\cos\left(P + \frac{\phi}{2}\right) + 3}{4\cos\left(\frac{2\varphi+\pi}{4}\right)} + \frac{\cos(2P - \phi) - 2}{1 + \sqrt{2}\cos\left(\frac{\varphi}{2}\right)} - \frac{1}{4\sqrt{2}\cos\left(\frac{\varphi}{2}\right)} \right\} + \mathcal{O}(\lambda^3)\,, \\
\Delta E_{2,0}(P,\phi,\varphi) &= 4\sqrt{2}\cos\left(\frac{\varphi}{2}\right) - \lambda 2\cos(P) \\
&- \lambda^2 \left\{ \frac{\cos(P - \phi) + 1}{1 - \sqrt{2}\sin\left(\frac{\varphi}{2}\right)} + \frac{\cos(P + \phi) + 1}{1 + \sqrt{2}\sin\left(\frac{\varphi}{2}\right)} - \frac{2}{1 + \sqrt{2}\cos\left(\frac{\varphi}{2}\right)} + \frac{\cos(2P) - 1}{4\sqrt{2}\cos\left(\frac{\varphi}{2}\right)} \right\} + \mathcal{O}(\lambda^3)\,.
\end{aligned}
\tag{4.2.8}
$$

Again, $\Delta E_{3,0}$ is given by (4.2). The special case $\phi = \varphi$ and $P = 0$ of (4.2.8) was presented in [68].

Returning to the $\mathbb{Z}_3$-chain we observe that for $\phi = \varphi = \frac{\pi}{2}$ we have to use degenerate perturbation theory. This was not done before [91] but can easily implemented for $P = 0$ with the method of section 3.3 and was carried out in [91]. It is straightforward to verify the exact result (4.1.3b) which was first shown by [21] $\Delta E_{2,0}\left(\frac{\pi}{2}, \frac{\pi}{2}\right) = 4(1 - \lambda)$ up to order λ^8. Unfortunately, $P \neq 0$ is not yet accessible to perturbative computations because the lowest eigenvector of the potential has a very complicated P-dependence and becomes quite simple just for $P = 0$. Nevertheless, the fact that we are able to compute fairly high orders even in degenerate cases demonstrates the universality of the approach to perturbation expansions outlined in section 3.3.

Also for the higher excitations we must apply degenerate perturbation theory. The next simplest case are the states where two spins are different from zero. For general n, P, $-\frac{\pi}{2} < \varphi < \frac{\pi}{2}$ the space of the excitation with one spin flipped into charge sector Q_1 and another one flipped into charge sector Q_2 is spanned by the states

$$
\|t_j^{Q_1,Q_2}\rangle\rangle_P := \|Q_1 \underbrace{0\ldots0}_{j-1 \text{ times}} Q_2 0\ldots0\rangle\rangle_P\,, \qquad 1 \leq j \leq \begin{cases} N-1, & \text{if } Q_1 \neq Q_2; \\ \left[\frac{N}{2}\right], & \text{if } Q_1 = Q_2. \end{cases} \tag{4.2.9}
$$

Obviously, we will have to consider two cases: $Q_1 \neq Q_2$ and $Q_1 = Q_2$.

For $Q_1 \neq Q_2$ it is not obvious even for $n = 3$ how to diagonalize V in the space (4.2.9) in closed form although one can easily diagonalize it numerically for comparably long chains – for details see appendix A.

In the second case $Q_1 = Q_2$ one can diagonalize the potential V in the space (4.2.9) explicitly exploiting a connection to graph theory (see e.g. [80]). We shift the details of the computation to appendix A and now present just the result.

It turns out that in the case of two identical excitations one has to distinguish between even and odd momenta in terms of lattice sites. It is convenient to introduce a further abbreviation δ_P^N encoding this distinction:

$$\delta_P^N := 0\ , \quad \text{if } \frac{PN}{2\pi} \text{ odd}; \qquad\qquad \delta_P^N := 1\ , \quad \text{if } \frac{PN}{2\pi} \text{ even}. \tag{4.2.10}$$

The result of the calculation in appendix A for the eigenvectors of the potential V is:

$$\begin{aligned} \|\tau_k^{Q,Q}\rangle\rangle_P := \frac{2}{\sqrt{N}}\Bigg\{ &\sum_{j=1}^{[\frac{N}{2}]-1} \sin\left(\frac{(2k-\delta_P^N)\, j\, \pi}{N}\right) e^{-i\frac{P}{2}(j-1)} \|t_j^{Q,Q}\rangle\rangle_P \\ &+ \frac{\sqrt{2}}{\sqrt{3+(-1)^N}} \sin\left(\frac{(2k-\delta_P^N)\,[\frac{N}{2}]\,\pi}{N}\right) e^{-i\frac{P}{2}([\frac{N}{2}]-1)} \|t_{[\frac{N}{2}]}^{Q,Q}\rangle\rangle_P \Bigg\}. \end{aligned} \tag{4.2.11}$$

The final result for the first order expansion of the energy for these excitations is for $N \geq 3$:

$$\begin{aligned} \Delta E_{2Q,k}(P,\phi,\varphi) =& 2\left(\sum_{k=1}^{n-1} \bar{\alpha}_k (1-\omega^{Qk})\right) - 4\lambda \frac{\cos\left(\frac{P}{2} - \left(1-\frac{2Q}{n}\right)\phi\right)\cos\left(\frac{(2k-\delta_P^N)\pi}{N}\right)}{\sin\left(\frac{\pi Q}{n}\right)} \\ &+ \mathcal{O}(\lambda^2)\ , \qquad 1 \leq k \leq \left[\frac{N+\delta_P^N-1}{2}\right] \end{aligned} \tag{4.2.12}$$

For a few remarks on the second order see the end of appendix A.

4.3. Spectrum in the low-temperature phase

In this section we calculate the ground state energy and the lowest excitations in the low-temperature phase using perturbative expansions according to [23] around $\tilde{\lambda} = 0$ of the Hamiltonian (3.1.2). We restrict once again to the $\mathbb{Z}_3$-version of the chiral Potts model (3.1.2) with periodic boundary conditions $R = 0$ but impose no restrictions on the angles ϕ, φ. We present low-temperature expansions for the ground state energy and in particular the first translationally invariant energy gaps that before [82] had not been treated by perturbative methods because of high degeneracies.

In each charge sector Q of the low-temperature phase there is one unique ground state. For arbitrary n it is given by (3.2.2) provided that $-\frac{\pi}{2} \leq \phi \leq \frac{\pi}{2}$. For $n = 3$ (3.2.2) is the ground state if $-\pi \leq \phi \leq \pi$ and for $n = 4$ (3.2.2) is the ground state for $-\frac{5\pi}{6} \leq \phi \leq \frac{5\pi}{6}$. The excited states are more complicated and highly degenerate. The space of the first excitation is spanned by those states which have precisely two blocks of different spins. Furthermore, the values of the spins in these two blocks must have difference one. For fixed P, Q and $-\frac{\pi}{2} \leq \phi \leq \frac{\pi}{2}$ we can choose the following basis for the space of the first excitation:

$$|a_k^Q\rangle := \frac{1}{\sqrt{n}} \sum_{l=0}^{n-1} \omega^{l\cdot Q} \| \underbrace{(l+1 \bmod n)\ldots(l+1 \bmod n)}_{k \text{ times}} l \ldots l\rangle\rangle_P. \tag{4.3.1}$$

In order to perform explicit calculations we now specialize to $n = 3$ with $P = 0$. In [82] a 5th order low-temperature expansion of the groundstate energy per site e_0 was computed. Upon interchanging ϕ and φ it agrees with (4.2.6) as predicted by duality (theorem V). It is noteworthy that the expansion in powers of $\tilde{\lambda}$ of e_0 does not depend on the charge sector for large N. More precisely, the order $\tilde{\lambda}^k e_0^{(k)}$ of the free energy does not depend on the charge if $N > k$. However, ground state level crossings have been observed in [105, 66] which in the perturbative approach are due to the fact that for short chain length N high orders $\tilde{\lambda}^k$ $(k \geq N)$ do depend on the charge Q. These level crossings at fixed $\tilde{\lambda}$ in the massive phase were exploited in [66] to compute a critical exponent of the wave vectors by the argument introduced in [67]. For more details on the relation to perturbation series compare [82].

The calculation of the smallest gap $\Delta E_{Q,1}$ is more difficult. Let q be the projector onto the space spanned by the states $\mid a_k^Q\rangle$ (4.3.1). In this space, the potential acts as follows:

$$\begin{aligned}
q\tilde{r}(V)\mid a_1^Q\rangle &= -\frac{2}{\sqrt{3}}(2e^{\frac{i\varphi}{3}}\mid a_2^Q\rangle + e^{\frac{i\varphi}{3}}\omega^Q\mid a_{N-1}^Q\rangle) \\
q\tilde{r}(V)\mid a_k^Q\rangle &= -\frac{2}{\sqrt{3}}(2e^{\frac{i\varphi}{3}}\mid a_{k+1}^Q\rangle + 2e^{-\frac{i\varphi}{3}}\mid a_{k-1}^Q\rangle) \qquad 1 < k < N-1 \\
q\tilde{r}(V)\mid a_{N-1}^Q\rangle &= -\frac{2}{\sqrt{3}}(2e^{-\frac{i\varphi}{3}}\mid a_{N-2}^Q\rangle + e^{-\frac{i\varphi}{3}}\omega^{2Q}\mid a_1^Q\rangle).
\end{aligned} \tag{4.3.2}$$

In the limit $N \to \infty$ the eigenvector with lowest eigenvalue converges to

$$\frac{1}{\sqrt{N-1}}\sum_{k=1}^{N-1}\mid a_k^Q\rangle\,. \tag{4.3.3}$$

Using (4.3.2) and (4.3.3) we can calculate that for $N \to \infty$ and $\phi < \frac{\pi}{2}$

$$\begin{aligned}
\lim_{N\to\infty}\Delta E_{Q,1} =& 4\sqrt{3}\cos\left(\frac{\phi}{3}\right) - \tilde{\lambda}\frac{8}{\sqrt{3}}\cos\left(\frac{\varphi}{3}\right) \\
&+\tilde{\lambda}^2\left\{\frac{8\cos\left(\frac{\phi}{3}\right)\left(1+\cos\left(\frac{2\varphi}{3}\right)\right)}{3\sqrt{3}\left(3-4\cos\left(\frac{\phi}{3}\right)^2\right)} + \frac{4\left(2-\cos\left(\frac{2\varphi}{3}\right)\right)}{3\sqrt{3}\cos\left(\frac{\phi}{3}\right)}\right\} + \mathcal{O}(\tilde{\lambda}^3).
\end{aligned} \tag{4.3.4}$$

Comparing (4.3.4) with the corresponding high-temperature expansion (4.2.7) shows that up to the order calculated it coincides with $\Delta E_{1,0}(\lambda) + \Delta E_{2,0}(\lambda)$ at the dual point $\lambda = \tilde{\lambda}$ with ϕ, φ interchanged. Furthermore, one can argue that the finite-size corrections to (4.3.4) are of order N^{-2} [82]. This further supports the identification of (4.3.4) with the dual of a two-particle state. Of course, (4.3.4) holds only for $\phi < \frac{\pi}{2}$.

For $\phi \geq \frac{\pi}{2}$, the states (4.3.1) are not the first excited states any more. Now we have to consider the following states:

$$\begin{aligned}
\frac{1}{\sqrt{n}}\Big(&\|1\ldots1\;2\ldots2\ldots0\ldots0\rangle\!\rangle_P + \omega^Q\|2\ldots2\ldots1\ldots1\rangle\!\rangle_P \\
&+\ldots+\omega^{Q(n-1)}\|0\ldots0\ldots(n-1)\ldots(n-1)\rangle\!\rangle_P\Big).
\end{aligned} \tag{4.3.5}$$

Going through the same steps as before we find:

$$\begin{aligned}\lim_{N\to\infty}\Delta E_{Q,1} =&12\sin\left(\frac{\pi-\phi}{3}\right)-\tilde{\lambda}4\sqrt{3}\cos\left(\frac{\varphi}{3}\right)\\&-\tilde{\lambda}^2\frac{2}{\sqrt{3}}\left\{\frac{\cos\left(\frac{2\varphi}{3}\right)-2}{\cos\left(\frac{\phi}{3}\right)}+\frac{\cos\left(\frac{2\varphi}{3}\right)+1}{\cos\left(\frac{\pi-\phi}{3}\right)}\right\}+\mathcal{O}(\tilde{\lambda}^3),\quad \frac{\pi}{2}\le\phi<\pi.\end{aligned}\tag{4.3.6}$$

(4.3.6) coincides with $3\Delta E_{1,0}(\lambda)$ at the dual point $\lambda=\tilde{\lambda}$ with interchanged ϕ, φ in the corresponding high-temperature expansion (4.2.7) up to the order calculated.

For $\phi=\frac{\pi}{2}$ the states (4.3.1) and (4.3.5) are degenerate. However, for large N the dominant contribution comes from the states (4.3.5) such that (4.3.6) is valid for $\phi=\frac{\pi}{2}$ as well. At $\phi=\varphi=\frac{\pi}{2}$ this is in agreement with the exact result of [21]:

$$\lim_{N\to\infty}\Delta E_{Q,1}=6(1-\tilde{\lambda})\qquad\text{for }\ \phi=\varphi=\frac{\pi}{2}.\tag{4.3.7}$$

4.4. Evidence for quasiparticle spectrum

Due to the studies of [41] (see proposition I) and [103] one expects a quasiparticle picture for the *integrable* $\mathbb{Z}_3$-chiral Potts model. Extensive numerical studies [68, 66, 69] showed that this quasiparticle picture is neither linked to integrability nor restricted to the $\mathbb{Z}_3$-chain. Furthermore, we were able to argue in [91] that this quasiparticle picture is to be expected in a quite general situation. Here, we do not want to go into technical details. We first recall the main statement, then discuss its origin and its consequences.

By a $\mathbb{Z}_n$-quasiparticle spectrum we understand the obvious generalization of (4.1.4):

Def. V: ($\mathbb{Z}_n$-quasiparticle spectrum) A family of spin chain Hamiltonians H_N has a $\mathbb{Z}_n$-quasiparticle spectrum iff in the limit $N\to\infty$ the spectrum of the excitation operator (3.1.14) can be obtained by the following rules:

$$\Delta E_{Q,r}(P,\phi,\varphi)=\sum_{k=1}^{m_r}\mathsf{E}_k(P^{(k)}),\quad P=\sum_{k=1}^{m_r}P^{(k)}\ \mathsf{mod}\ 2\pi\,,\quad Q=\sum_{k=1}^{m_r}Q^{(k)}\ \mathsf{mod}\ n\tag{4.4.1}$$

with m fundamental quasiparticles carrying energy $\mathsf{E}_1(P)$ to $\mathsf{E}_m(P)$ and charge $Q^{(1)}$ to $Q^{(m)}$.

Now the precise statement is:

Proposition II: *Let H_N be a nearest neighbour interaction spin chain Hamiltonian of the form $H_N=H_0+\lambda V$ such that H_N conserves $\mathbb{Z}_n$-charge for all λ. Assume that H_0 has a $\mathbb{Z}_n$-quasiparticle spectrum with $n-1$ fundamental particles of charge $Q^{(j)}=j$ ($j\neq 0$) and Brillouin zones $[0,2\pi]$. Assume furthermore that the perturbation series of the fundamental particles converge for $\lambda<\lambda_0$.*

Then for $\lambda<\lambda_0$ the limit $N\to\infty$ of the complete excitation spectrum of H_N exists and it is a $\mathbb{Z}_n$-quasiparticle spectrum with $n-1$ fundamental particles of charge $Q^{(j)}=j$ ($j\neq 0$) and Brillouin zones $[0,2\pi]$. ∎

Remarks:

1) For the $\mathbb{Z}_n$-chiral Potts model (3.1.1) with the parameterization (3.1.12) the assumptions of proposition II can be easily checked except for a non-trivial radius of convergence which we shall check for the $\mathbb{Z}_3$-chain below in section 4.5. However, proposition II also covers more general cases, e.g. also the Hamiltonians (2.4.5), (2.4.6) and (2.4.9).
2) Due to the assumptions the only overlap between proposition I and proposition II is the trivial point $\lambda = 0$ on the superintegrable line of the $\mathbb{Z}_3$-chain.

Recall that one may expect to interpret the energy bands as continuous spectrum in the weak limit of the Hamiltonian [69, 91] and that the single-particle excitations (4.2.2) lead to point spectrum. The normalization factors $\frac{2}{\sqrt{N}}$ for the two-particle states in (4.2.11) demonstrate that these states tend to zero for $N \to \infty$ and will therefore not give rise to proper eigenvectors. Furthermore, comparing (4.2.12) with the first order expansion for the single-particle states (4.2.3) one observes that this first order expansion of the two-particle excitations is in agreement with the quasiparticle rule (4.4.1). Up to first order the composite particle states satisfy either $2\Delta E_{Q,0}(P,\phi,\varphi) < \Delta E_{2Q,k}(2P,\phi,\varphi) < 2\Delta E_{Q,0}(P+2\pi,\phi,\varphi)$ or $2\Delta E_{Q,0}(P,\phi,\varphi) > \Delta E_{2Q,k}(2P,\phi,\varphi) > 2\Delta E_{Q,0}(P+2\pi,\phi,\varphi)$ depending on which one of the single-particle energies is larger. Thus, the two-particle states do indeed lie inside the energy band of two single-particle states and the boundaries are not included. Even more, we can see from (4.2.12) that the two-particle states become dense in this energy band for $N \to \infty$.

The proof of proposition II relies on the interaction in the Hamiltonian (3.1.1) being very short ranged – in fact, only among nearest neighbours. In the massive high-temperature phase there is no spontaneous order and the correlation length is finite. Thus, if one puts two excitations of 'short' chains with a sufficient separation on a longer chain, the interaction will be negligible. In pictures:

$$\underset{E_1,P_1,Q_1}{\overbrace{\bullet\!-\!\!-\!\bullet\cdots\cdots\bullet\!-\!\!-\!\bullet}^{N}} \otimes \underset{E_2,P_2,Q_2}{\overbrace{\bullet\!-\!\!-\!\bullet\cdots\cdots\bullet\!-\!\!-\!\bullet}^{M}} \underset{N,M\to\infty}{\longrightarrow} \underset{E_1+E_2,P_1+P_2,Q_1+Q_2}{\overbrace{\bullet\!-\!\!-\!\bullet\cdots\cdots\bullet\!-\!\!-\!\bullet}^{N+M}} . \tag{4.4.2}$$

For example, putting one single-particle excitation one the left half of the chain and another on the right half will approximate a two-particle excitation.

In order to make the derivation rigorous one has to show the vanishing of boundary terms in (4.4.2). This can indeed be done using e.g. perturbative arguments [91]. Because this is very technical we do not want to recall the complete argument here. Just note that the crucial point is that the momentum eigenstates have normalization factors $N^{-\frac{1}{2}}$, $M^{-\frac{1}{2}}$. Any operator acting only at boundaries yields only a finite part of these states in contrast to the operators T_N and $\Delta H_N^{(n)}$ which act on the complete chain and yield complete momentum eigenstates. The finite pieces of momentum eigenstates are suppressed by the normalization factors $N^{-\frac{1}{2}}$ in the infinite chain length limit.

Note that boundary terms are substantial for conformally invariant systems with long ranged correlations. Also in the low-temperature phase boundary terms play an important rôle because the free part of the Hamiltonian depends on the difference of neighbouring spins [82]. Thus, proposition II applies neither to critical points where one might have conformal invariance nor to the low-temperature phase.

We have not assumed the Hamiltonian to be hermitean. In particular, the quasiparticle picture should also be valid for $\phi \in \mathbb{C}$ as long as the single-particle excitations exist and converge. This is indeed supported by numerical calculations [126].

The argument proving the quasiparticle structure can be refined in order to give an upper estimate for the rate of convergence in N of the energy of a k-particle state. As an approximation to a k-particle state for kN sites, total energy E_{tot} and total momentum P we may take the k-fold tensor product of single-particle states

$$\|kN; E_{\text{tot}}\rangle\rangle_{\,P} := \|N; E_1\rangle\rangle_{\,P_1} \otimes \ldots \otimes \|N; E_k\rangle\rangle_{\,P_k} \tag{4.4.3}$$

with $E_{\text{tot}} = \sum_{l=1}^{k} E_l$, $P = \sum_{l=1}^{k} P_l$. Now, the deviation from the limit $N \to \infty$ is given by:

$$_{P}\langle\langle kN; E_{\text{tot}}\|\, \Delta H_{kN}^{(n)} \|kN; E_{\text{tot}}\rangle\rangle_{\,P} - E_{\text{tot}} = \prod_{l=1}^{k} {}_{P_l}\langle\langle N; E_l\|\, \mathcal{O}(\Delta H_N)\|N; E_l\rangle\rangle_{\,P_l} = \mathcal{O}(N^{-k}) \tag{4.4.4}$$

where $\mathcal{O}(\Delta H_N)$ is some operator that acts only at sites 1 and N. The first equality simply uses the definition of the scalar product in tensor products. The last equality is more profound and due to the fact that operators acting only at boundaries of the chain are suppressed by N^{-1} due to the normalization factor in the finite fourier transformation for momentum eigenstates. This general argument is confirmed by our results for the two-particle states. Expanding $\cos(x) = 1 - \frac{1}{2}x^2 + \mathcal{O}(x^4)$ we can read off from (4.2.12) that the first order correction of the rth two-particle state with respect to the boundary of the energy band behaves as N^{-2} which agrees with (4.4.4).

In summary, we have the following results on the finite-size effects:

1) Single-particle states converge exponentially in N as long as the corresponding perturbation series converge since the rth orders are independent of N if $N > r+1$.
2) The deviation of the energy of a k-particle state ($k > 1$) from the limit is at most of order N^{-k} for $N \to \infty$. Note that consequently, the N-dependence of some energy eigenvalue yields only a lower bound on the number k of particles involved.

In particular, the *energy* of any state remains unchanged to order $\frac{1}{N}$ in a finite-size system. Thus, the only modification in (4.4.1) at order $\frac{1}{N}$ in the massive high temperature phase is a discretization of the momentum (and possible minor modifications of the Brillouin zones and selection rules [103]).

Note that the proof of the vanishing of boundary terms as sketched above and presented in detail in [91] also directly applies to the Hamiltonian (3.1.1) itself. So far, we have restricted ourselves to periodic boundary conditions but one could also use cyclic, twisted or even free boundary conditions. Our argument shows that all these different choices lead to the same spectrum in the limit $N \to \infty$. In particular, our results are valid for all choices of boundary conditions and one is free to choose those which seem most appropriate, e.g. one can leave the ends of the chain open instead of the unnatural end-identification for a realistic physical system.

Again, this observation for the massive high-temperature phase is to be contrasted with other situations. In particular, at the second order phase transition $\phi = \varphi = 0$, $\lambda = 1$ the correlation length becomes infinite and the boundary terms are very important [37, 74, 90]. Even in the massive low-temperature phase one observes long range order and boundary terms cannot be neglected [82].

Similarly one can directly argue that in the low-temperature regime all charge sectors are degenerate for $N \to \infty$, at least if the perturbation expansion converges [82]. That means that in the massive low-temperature regime the thermodynamic limit does not depend on Q. The independence of the spectrum of the charge Q in the low-temperature regime is also expected due to duality (theorem V) because in the massive high-temperature phase it does not depend on the boundary conditions R.

So far we have not addressed the question of whether the fundamental particles satisfy a Pauli principle or not – note that the above discussion is intrinsically insensitive to a Pauli principle because the limit was defined such that the spectrum forms a closed set. Nevertheless, for the special case $n = 3$ and $\phi = \varphi = \frac{\pi}{2}$, eq. (4.4.1) was obtained in [41] supplemented with the Pauli principle. Fortunately, due to (4.2.12), we have some control over the finite-size dependence of the scattering states of two identical particles in the general case. Up to first order in λ these finite-size effects do essentially neither depend on the charge Q nor on the number of states n for periodic boundary conditions. Therefore, the nature of the fundamental excitations can be determined by looking at one particular choice of Q and n. However, for $n = 2$ one obtains the Ising model where it is well-known that the excitation spectrum can be explained in terms of one fundamental *fermion* (see e.g. [104]). This indicates that the fundamental excitations for general n should behave similar to fermions. In particular, for a scattering state of two identical excitations i and j the momenta must satisfy $P_i \neq P_j$. In a scattering state of two *different* fundamental particles these two fundamental particles can easily be distinguished because they carry different $\mathbb{Z}_n$-charges. Therefore, two different particles should not be subject to a Pauli principle (like it is the case for two different non-interacting fermions).

From theorem V we conclude that the quasiparticle interpretation for the high-temperature phase of the general $\mathbb{Z}_n$-chiral Potts quantum chain given by proposition II can be pulled over to the low-temperature phase. The duality transformation interchanges charge sector Q and boundary conditions R. Thus, the ground state of the high-temperature phase is mapped to periodic boundary conditions $R = 0$ in the low-temperature phase. However, the fundamental excitations are mapped to different boundary conditions corresponding to the charge sectors $R \in \{1, \ldots n-1\}$. Therefore we observed only composite particle states in section 4.3.

4.5. Convergence of single-particle excitations

As far as the quasiparticle picture of proposition II is concerned the main open question is the convergence of the single-particle states, or equivalently the existence of the limits $N \to \infty$ of the corresponding eigenvalues of the Hamiltonian. We have argued in section 4.2

that convergence of the perturbation expansions is sufficient to guarantee the existence of the limits $N \to \infty$. Therefore we will discuss the radius of convergence for the perturbation expansion of the single-particle excitations in this section.

The potential for $\Delta H_N^{(n)}$ as defined in (3.1.1) and (3.1.14) is unbounded if N is not fixed. Thus, we have to apply the Kato-Rellich theory of regular perturbations. Reviews of this subject can be found e.g. in the monographs [117, 100]. The main results we are going to use were originally published in [118, 99]. The theory of Kato and Rellich applies in particular to operators of the form $H(\lambda) = H_0 + \lambda V$.

Suppose that the single-particle eigenvalues ΔE have a non-zero distance from the scattering eigenvalues (the continuous spectrum) at $\lambda = 0$. Then it is clear from the discussion in the previous sections that these eigenvalues are non-degenerate and isolated. In particular, the resolvent $(\Delta H_N^{(n)}(\lambda) - z)^{-1}$ is bounded for $|\Delta E - z| > 0$. Restricting to the hermitean case, this is sufficient to guarantee that the $\Delta H_N^{(n)}(\lambda)$ are an analytic family in the sense of Kato. In this case, the Kato-Rellich theorem ([117] Theorem XII.8) may be used to guarantee a non-zero radius of convergence $r_0 > 0$ for the single-particle eigenvalues of $\Delta H_N^{(n)}(\lambda)$.

In order to obtain explicit estimates of the radius of convergence one needs the inequality

$$\|V \,|a\rangle\,\| \leq \mathcal{V}\|H_0 \,|a\rangle\,\| + \mathcal{K}\|\,|a\rangle\,\| \tag{4.5.1}$$

on $\mathcal{D}(H_0)$ which in our case is dense in the the complete Hilbert space $\mathcal{H}$. Then, the isolated point eigenvalues of $H(\lambda)$ are convergent at least for

$$\lambda < r_1 := \mathcal{V}^{-1} \tag{4.5.2}$$

as long as these eigenvalues *do not come in contact with continuous spectrum* [99]. On the one hand this criterion is very simple, on the other hand one must estimate not only the constant $\mathcal{V}$ but also examine the level crossings between single-particle excitations and scattering states. There is another estimate r_2 that guarantees the separation of eigenvalues as well but gives smaller radii of convergence. For self-adjoint H_0 with isolated eigenvalue $E_0^{(0)}$ where the nearest eigenvalue $E_1^{(0)}$ has distance $\epsilon := |E_1^{(0)} - E_0^{(0)}|$ ($\epsilon^{-1} = \|g(E_0^{(0)})\|$) the perturbation expansion of $E_0(\lambda)$ is convergent for

$$\lambda < r_2 := \frac{\epsilon}{2\left(\mathcal{K} + \mathcal{V}(|E_0^{(0)}| + \epsilon)\right)} \tag{4.5.3}$$

and there are no crossings with neighbouring levels. In order to compare the estimates (4.5.2) and (4.5.3) let us assume $\mathcal{K} = 0$ and $|E_0^{(0)}| = \epsilon$. For this almost optimal case one has $r_1 = 4r_2$ showing that the criterion (4.5.3) is much more restrictive.

Let us now apply these general results to the present case of $\mathbb{Z}_n$-spin quantum chains. For non-degenerate single-particle eigenvalues the Kato-Rellich theorem can be applied to guarantee a positive radius of convergence r_0. Then we know from section 4.4 that the spectrum of $\Delta H_N^{(n)}(\lambda)$ is a quasiparticle spectrum for $\lambda < r_0$. This fact can be used to calculate the constant $\mathcal{V}$ and obtain explicit estimates r_1 (where level crossings still have to be discussed) or r_2. One can obtain the estimate (4.5.1) with $\mathcal{K} = 0$ using Schwarz' inequality:

$$\mathcal{V} := \sup_{|a\rangle \in \mathcal{H}} \frac{\langle a|\ \Delta V\ |a\rangle}{\|\Delta H_{N,0}^{(n)}\ |a\rangle\ \|}. \tag{4.5.4}$$

In general, this supremum need not be finite but then it is very difficult to ensure convergence at all. In our case, the important observation is that due to the quasiparticle picture we can evaluate (4.5.4) exclusively from the single-particle excitations. To see this one performs a first order expansion in λ for any composite particle state, compares coefficients and uses the quasiparticle property to expand the expectation values of $\Delta H_{N,0}^{(n)}$ and ΔV in single-particle excitations. Thus, $\mathcal{V}$ can be calculated as

$$\mathcal{V} = \max_{Q,P} \frac{{}_P\langle\langle s^Q \|\ \Delta V \| s^Q\rangle\rangle\ {}_P}{\|\Delta H_{N,0}^{(n)} \| s^Q\rangle\rangle\ {}_P \|}. \tag{4.5.5}$$

In order to implement this program explicitly we specialize to the case of $\mathbb{Z}_3$ with the parameterization (3.1.12). At $\lambda = 0$ both single-particle eigenvalues are isolated for $-\frac{\pi}{2} < \varphi < \frac{\pi}{2}$. This guarantees a non-zero radius of convergence r_0.

The simplest case is the parity conserving case $\phi = \varphi = 0$. Here, the maxima are located at zero momentum $P = 0$ and both charge sectors are degenerate. Furthermore, we have $\|\Delta H_{N,0}^{(3)} \| s^Q\rangle\rangle\ {}_0\| = \epsilon = E_0^{(0)}$. From (4.2.7) at $\phi = \varphi = 0$ we can therefore read off $\mathcal{V} = \frac{2}{3}$, or in terms of radii of convergence

$$r_1 = \frac{3}{2}, \qquad r_2 = \frac{3}{8}, \qquad \text{for} \quad n = 3,\ \phi = \varphi = 0. \tag{4.5.6}$$

$r_2 = 0.375$ is certainly too small (for more details see [91]).

For general angles $0 \leq \varphi < \pi$, the free part of the Hamiltonian $\|\Delta H_{N,0}^{(3)} \| s^Q\rangle\rangle\ {}_0\|$ is minimized for $Q = 1$ and the potential ${}_P\langle\langle s^Q \|\ \Delta V \| s^Q\rangle\rangle\ {}_P$ is maximal for $P = \frac{\phi}{3}$. Thus, we read off from (4.2.7) $\mathcal{V} = \left(\sqrt{3}\sin\left(\frac{\pi-\varphi}{3}\right)\right)^{-1}$. The relevant distance ϵ in the spectrum at $\lambda = 0$ is given by the distance from the $Q = 2$ fundamental particle to a state of k particles with $Q = 1$ where k depends on φ. Note that k must be equal $2 = Q \bmod 3$. Thus, one has $\epsilon = 4|k\sin\left(\frac{\pi-\varphi}{3}\right) - \sin\left(\frac{\pi+\varphi}{3}\right)|$ and $E_0^{(0)} = 4\sin\left(\frac{\pi-\varphi}{3}\right)$. This amounts to the following radii

$$r_1 = \sqrt{3}\sin\left(\frac{\pi-\varphi}{3}\right), \qquad r_2 = \min_k \frac{\sqrt{3}\sin\left(\frac{\pi-\varphi}{3}\right)|k\sin\left(\frac{\pi-\varphi}{3}\right) - \sin\left(\frac{\pi+\varphi}{3}\right)|}{2\left(\sin\left(\frac{\pi-\varphi}{3}\right) + |k\sin\left(\frac{\pi-\varphi}{3}\right) - \sin\left(\frac{\pi+\varphi}{3}\right)|\right)} \tag{4.5.7}$$

for $n = 3$, $0 \leq \varphi < \pi$. For $0 \leq \varphi \leq \frac{\pi}{2}$ the closest state is a two-particle state, i.e. $k = 2$. For $\varphi \to \frac{\pi}{2}$ the situation is contrary to that at $\phi = \varphi = 0$. The $Q = 2$ particle state becomes degenerate with two $Q = 1$ scattering states at $\varphi = \frac{\pi}{2}$ such that the radius of convergence must tend to zero for $\varphi \to \frac{\pi}{2}$. Whereas r_2 has precisely this property, r_1 tends to $0.866\ldots$ which is certainly too large.

Because for small φ we would prefer the large radius of convergence r_1 but at $\varphi \approx \frac{\pi}{2}$ this is much too large and r_2 seems more appropriate we have to enhance the estimate given by r_1 by a discussion of level crossings between single-particle states and scattering states. For $0 \leq \varphi < \frac{\pi}{2}$ the first level crossing of this kind will take place between the $Q = 2$ single-particle excitation and a two $Q = 1$ particles scattering state.

It is very difficult to determine those values of λ explicitly and precisely where they take place. Therefore, we will use the first order approximation of the perturbation expansion. We are looking for those values of λ where a single point P exists such that $x(k) := k\Delta E_{1,0}(\frac{P}{k}, \phi, \varphi) - \Delta E_{2,0}(P, \phi, \varphi)$ (with $k \equiv 2 \bmod 3$) vanishes. The fact that we are looking for no real crossings but $x(k) = 0$ implies $\frac{\mathrm{d}x(k)}{\mathrm{d}P} = 0$. Inserting (4.2.7) and (4.2) up to first order leads to the condition

$$\sin\left(\frac{P}{k} - \frac{\phi}{3}\right) = \sin\left(P + \frac{\phi}{3}\right) \tag{4.5.8}$$

Eq. (4.5.8) has a solution

$$P = \frac{k\pi}{k+1} \tag{4.5.9}$$

that does not depend on ϕ. Now we can solve the linear equation $x(k)\mid_{\lambda_0} = 0$ for the value λ_0. One obtains

$$\lambda_0(k) = \sqrt{3}\frac{\sin\left(\frac{\pi+\varphi}{3}\right) - k\sin\left(\frac{\pi-\varphi}{3}\right)}{\cos\left(\frac{k\pi}{k+1} + \frac{\phi}{3}\right) - k\cos\left(\frac{\pi}{k+1} - \frac{\phi}{3}\right)} \tag{4.5.10}$$

The $k = 2$ special case of (4.5.7) – (4.5.10) was discussed in [91].

Fig. 2 shows a plot of the estimates (4.5.7) and (4.5.10) for the self-dual case $\varphi = \phi$. Note that r_1 and r_2 are independent of ϕ. However, we have assumed that the Hamiltonian is hermitean and therefore ϕ must be real.

For completeness we have also included an estimate for the boundary of the massive high-temperature phase in Fig. 2. At this boundary, levels of the $Q = 1$ particle with generically non-zero momentum cross with the ground state. Its explicit location has been obtained estimating the minimum of the dispersion relation (4.2.7) with $P = \frac{\phi}{3}$ and solving the second order approximation $\Delta E_{1,0}(\frac{\phi}{3}, \phi, \phi) = 0$ for λ. This is a slightly modified version of the estimate already proposed in [97] where we have used the second order because it gives good agreement with exactly known points.

For a detailed discussion of Fig. 2 in the interval $0 \leq \varphi \leq \frac{\pi}{2}$ see [91].

The level crossings transition λ_0 divides the massive high-temperature phase of the $\mathbb{Z}_3$-chiral Potts model into two parts which we label IIa and IIb. Note that above the super-integrable line $\varphi = \frac{\pi}{2}$ there are infinitely many 'windows' of type IIa in which the $Q = 2$ quasiparticle exists in the entire Brillouin zone $[0, 2\pi]$. At those points where the $Q = 2$ fundamental particle crosses k $Q = 1$ particle states ($k \equiv 2 \bmod 3$) already for $\lambda = 0$, the radii of convergence become zero. The first crossing of this kind takes places at $\varphi = \frac{\pi}{2}$ with a two-particle state. The crossings and consequently also the 'windows' accumulate for $\varphi \to \pi$. Note that for $\varphi \geq \frac{\pi}{2}$ the estimates r_2 and λ_0 follow each other closely, i.e. the estimate r_2 is already close to optimum.

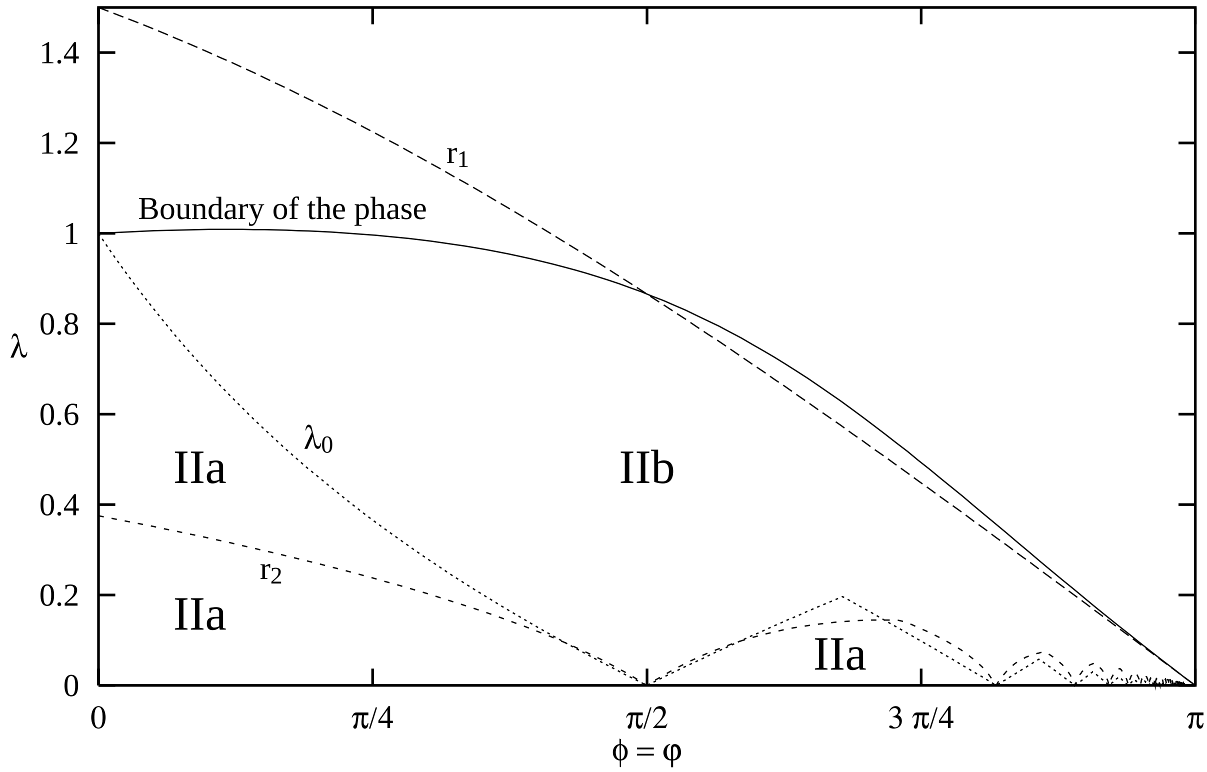

Fig. 2: Radii of convergence and boundary of the massive high-temperature phase for the hermitean $\mathbb{Z}_3$-chain. r_1 is an estimate ensuring convergence if *no level crossings between point and continuous spectrum occur.* The estimate r_2 also ensures the absence of level crossings. The perturbation series are definitely convergent for $\lambda < r_2$ although the true radius of convergence is larger. It extends until the value λ_0 where the first level crossings between fundamental quasiparticles and scattering states occur.
Note that r_1 and r_2 are independent of ϕ whereas for λ_0 we put $\varphi = \phi$.

In part IIa the derivation of the quasiparticle picture is rigorous. Thus, in regime IIa the spectrum is a quasiparticle spectrum with two fundamental particles existing for all momenta. In [69] we have presented numerical evidence that regime IIb probably also exhibits a quasiparticle spectrum with two fundamental particles where the $Q = 2$ particle has the unusual property that it exists only in a limited range of the momentum P. At $\varphi = \phi = \frac{\pi}{2}$ this statement is given by proposition I. We expect that the idea to approximate multi-particle states by putting single-particle states of 'small' chains with a sufficient separation on a longer chain and to use the finite correlation length in order to ensure vanishing of boundary terms (which we cannot show directly like in [91] any more) will apply also in regime IIb for general angles ϕ, φ. However, in contrast to section 4.4 we loose control over the fundamental $Q = 2$ excitation because the perturbation series does not converge any more and there is no guarantee for the completeness of this construction. At least it is plausible to still expect a quasiparticle spectrum in regime IIb with two fundamental particles of which the $Q = 2$ particle may have a Brillouin zone that is smaller than the interval $[0, 2\pi]$.

Tout cela est d'une grande beauté et d'une extrême importance, mais malheureusement nous ne le comprenons pas. Nous ne comprenons ni l'hypothèse de Planck sur les vibrateurs, ni l'exclusion des orbits non stationnaires, et nous ne voyons pas, dans la théorie de Bohr, comment, en fin de compte, la lumière est produite. Car, il faut bien l'avouer, la mécanique des quanta, la mécanique des discontinuités, doit encore être faite.

H.A. Lorentz in "L'ancienne et la nouvelle mécanique" (1925)

5. Correlation functions

In recent papers a systematic investigations of the correlation functions of the $\mathbb{Z}_3$-chiral Potts model in the massive phases has been started. First, a non-vanishing wave vector has been predicted in [66, 105] for the massive low-temperature phase and its critical exponent was calculated from level crossings. Below we wish to present the direct computations of the correlation functions of [82, 69, 91]. Note also that for the massless phases around $\lambda \sim 1$ of the $\mathbb{Z}_3$-chain correlation functions have been derived in [3] using results from conformal field theory.

5.1. Correlation functions of the high-temperature phase

In this section we study correlation functions for the $\mathbb{Z}_3$-chiral Potts model perturbatively. Before defining correlation functions, we first note that the two-point functions are translationally invariant because the groundstate $|\, v\rangle$ is translationally invariant:

$$\begin{aligned} \langle v|\ \Gamma^{+}_{x+r}\Gamma_r\ |v\rangle &= \langle v|\ \Gamma^{+}_{x+1}\Gamma_1\ |v\rangle\ , \\ \langle v|\ \sigma^{+}_{x+r}\sigma_r\ |v\rangle &= \langle v|\ \sigma^{+}_{x+1}\sigma_1\ |v\rangle\,. \end{aligned} \tag{5.1.1}$$

Thus, it makes sense to define the correlation function for an operator Ξ by the following expression:

$$C_\Xi(x) := \frac{\langle v|\ \Xi^{+}_{x+1}\Xi_1\ |v\rangle}{\langle v\,|\,v\rangle} - \frac{\langle v|\ \Xi^{+}_{x+1}\ |v\rangle\,\langle v|\ \Xi_1\ |v\rangle}{\langle v\,|\,v\rangle^{\,2}} \qquad 0 \le x < \frac{N}{2} \tag{5.1.2}$$

where $|\, v\rangle$ is the eigenvector of the Hamiltonian to lowest energy. Here, we do not assume that $|\, v\rangle$ is normalized to one and have therefore included the proper normalization factors in (5.1.2).

The operator Ξ for the $\mathbb{Z}_3$-chiral Potts model can be either Γ or σ. (For $n > 3$ also different powers of these operators may be interesting.) The correlation functions of the operators Γ_x and σ_x have the property

$$\begin{aligned} C_\Gamma(-x) &= C_\Gamma(x)^*\ , \\ C_\sigma(-x) &= C_\sigma(x)^* = C_\sigma(x) \end{aligned} \tag{5.1.3}$$

such that it makes sense to restrict to positive x. Note that (5.1.3) follows by complex conjugation using (5.1.1). Explicit calculations show the validity of (5.1.1) and (5.1.3) as well.

Let us now turn to the explicit computation of correlation functions for the $\mathbb{Z}_3$-chain. In order to be able to calculate the correlation functions we need to know the groundstate $|\, v\rangle$. We will calculate it from the free ground state $|\,\mathrm{GS}\rangle$ using the perturbation expansion (3.3.5). We should stress again that although we assume the free groundstate $|\,\mathrm{GS}\rangle$ to be normalized to 1, this is not necessarily true for the complete state $|\, v\rangle$. The expansion of the groundstate $|\, v\rangle$ provides us with an expansion for the correlation functions in powers of λ

$$C_\Xi(x) = \sum_{\nu=0}^{\infty} \lambda^\nu C_\Xi^{(\nu)}(x)\,. \tag{5.1.4}$$

Note that according to (3.3.5) a kth order expansion of the groundstate yields a $k+1$th order expansion of the groundstate energy as a byproduct.
The operator Γ_x creates charge such that charge conservation implies $\langle v \mid \Gamma_x^+ \mid v\rangle = \langle v \mid \Gamma_x \mid v\rangle = 0$ for all x. Thus

$$C_\Gamma(x) = \frac{\langle v \mid \Gamma_{x+1}^+ \Gamma_1 \mid v\rangle}{\langle v \mid v\rangle}. \tag{5.1.5}$$

Here we omit the intermediate steps and present just the final results of the computations. The interested reader may find some more details in [91].
The final result for the expansion of $C_\sigma(x)$ is

$$\begin{aligned}
C_\sigma^{(0)}(x) =& C_\sigma^{(1)}(x) = 0\,,\\
C_\sigma^{(2)}(x) =& \frac{1}{3\mathcal{C}^2}\left\{\delta_{x,0} + \frac{\delta_{x,1}}{4}\right\}, \qquad C_\sigma^{(3)}(x) = \frac{\cos(\phi)}{9\mathcal{C}^3}\left\{\delta_{x,0} + \frac{\delta_{x,1}}{4}\right\},\\
C_\sigma^{(4)}(x) =& \frac{1}{27\mathcal{C}^2}\Bigg\{ - \delta_{x,0}\left(\frac{2(1-10\mathcal{C}^2)}{\mathcal{R}^2} + \frac{3}{2\mathcal{C}^2}\right) + \delta_{x,1}\left(\frac{1+20\mathcal{C}^2}{3\mathcal{R}^2} - \frac{1}{\mathcal{C}^2}\right)\\
&\qquad + \delta_{x,2}\left(\frac{2(1+2\mathcal{C}^2)}{3\mathcal{R}^2} + \frac{1}{16\mathcal{C}^2}\right)\Bigg\}.
\end{aligned} \tag{5.1.6}$$

For the other correlation function $C_\Gamma(x)$ one finds the following final result

$$\begin{aligned}
C_\Gamma^{(0)}(x) =& \delta_{x,0}\,, \qquad C_\Gamma^{(1)}(x) = \delta_{x,1}\frac{e^{i\frac{\phi}{3}}}{3\mathcal{C}}\,, \qquad C_\Gamma^{(2)}(x) = \frac{1}{6\mathcal{C}^2}\left\{\delta_{x,1}\frac{e^{-i\frac{2\phi}{3}}}{2} + \delta_{x,2}e^{i\frac{2\phi}{3}}\right\},\\
C_\Gamma^{(3)}(x) =& \frac{1}{54\mathcal{C}}\left\{ - \delta_{x,1}\, e^{i\frac{\phi}{3}}\left(\frac{1}{\mathcal{C}^2} + \frac{8}{\mathcal{R}}\right) + \delta_{x,2}\, e^{-i\frac{\phi}{3}}\left(\frac{2}{\mathcal{C}^2} - \frac{8}{\mathcal{R}}\right) + \delta_{x,3}\frac{5e^{i\phi}}{\mathcal{C}^2}\right\}\\
C_\Gamma^{(4)}(x) =& \frac{1}{81\mathcal{C}^2}\Bigg\{ - \delta_{x,1}\left(e^{i\frac{4\phi}{3}} + 4e^{-i\frac{2\phi}{3}}\right)\left(\frac{9}{16\mathcal{C}^2} + \frac{3}{\mathcal{R}}\right)\\
&\quad + \delta_{x,2}\left(\frac{8e^{i\frac{2\phi}{3}}(19\mathcal{C}^2-4)}{3\mathcal{R}^2} + \frac{3e^{-i\frac{4\phi}{3}} - 20e^{i\frac{2\phi}{3}}}{8\mathcal{C}^2} - \frac{3e^{-i\frac{4\phi}{3}}}{\mathcal{R}}\right)\\
&\quad + \delta_{x,3}\left(\frac{40\mathcal{C}^2-7}{\mathcal{R}^2} + \frac{9}{4\mathcal{C}^2}\right) + \delta_{x,4}\frac{35e^{i\frac{4\phi}{3}}}{8\mathcal{C}^2}\Bigg\}
\end{aligned} \tag{5.1.7}$$

It is easy to see that $C_\Gamma^{(k)}(x)$ and $C_\sigma^{(k)}(x)$ are independent of N if $N > 2k$ and $x \leq k$.

$C_\sigma(x)$ is real and positive for all values of ϕ and φ up to the order calculated. However, it is not easy to read off from (5.1.6) what might be the form for large x. Thus, we specialize to $\phi = \phi = \frac{\pi}{2}$ and calculate two further orders for $C_\sigma(x)$:

$$\begin{aligned} C_\sigma^{(0)}(x) =& C_\sigma^{(1)}(x) = C_\sigma^{(3)}(x) = C_\sigma^{(5)}(x) = 0 \ , \\ C_\sigma^{(2)}(x) =& \frac{1}{9}\left\{4\delta_{x,0} + \delta_{x,1}\right\} \ , \\ C_\sigma^{(4)}(x) =& \frac{1}{81}\left\{5\delta_{x,0} + 2\delta_{x,2}\right\} \ , \\ C_\sigma^{(6)}(x) =& \frac{1}{6561}\left\{190\delta_{x,0} - 13\delta_{x,1} + 38\delta_{x,2} + 60\delta_{x,3}\right\} . \end{aligned} \tag{5.1.8}$$

$C_\Gamma(x)$ in general has a non-vanishing imaginary part and therefore is worth while being considered in more detail. Thus, we specialize again to the superintegrable case $\phi = \varphi = \frac{\pi}{2}$ [4]) and obtain after calculating two further orders

$$\begin{aligned} C_\Gamma^{(0)}(x) =& \delta_{x,0} \ , \qquad\qquad C_\Gamma^{(1)}(x) = \delta_{x,1}\left(\frac{1}{3} + i\frac{\sqrt{3}}{9}\right) \ , \\ C_\Gamma^{(2)}(x) =& \frac{1}{18}\left\{\delta_{x,1} + 2\delta_{x,2}\right\} + i\frac{\sqrt{3}}{18}\left\{-\delta_{x,1} + 2\delta_{x,2}\right\} \ , \\ C_\Gamma^{(3)}(x) =& \frac{1}{81}\left\{4\delta_{x,1} + 10\delta_{x,2}\right\} + i\frac{\sqrt{3}}{243}\left\{4\delta_{x,1} - 10\delta_{x,2} + 20\delta_{x,3}\right\} \ , \\ C_\Gamma^{(4)}(x) =& \frac{1}{1458}\left\{27\delta_{x,1} + 18\delta_{x,2} + 210\delta_{x,3} - 70\delta_{x,4}\right\} + i\frac{\sqrt{3}}{1458}\left\{-27\delta_{x,1} + 18\delta_{x,2} + 70\delta_{x,4}\right\} \ , \\ C_\Gamma^{(5)}(x) =& \frac{1}{2187}\left\{45\delta_{x,1} + 108\delta_{x,2} + 252\delta_{x,4} - 126\delta_{x,5}\right\} \\ & + i\frac{\sqrt{3}}{2187}\left\{15\delta_{x,1} - 36\delta_{x,2} - 14\delta_{x,3} + 84\delta_{x,4} + 42\delta_{x,5}\right\} \ , \\ C_\Gamma^{(6)}(x) =& \frac{1}{39366}\left\{381\delta_{x,1} + 214\delta_{x,2} + 2314\delta_{x,3} + 784\delta_{x,4} + 2310\delta_{x,5} - 1848\delta_{x,6}\right\} \\ & + i\frac{\sqrt{3}}{39366}\left\{-381\delta_{x,1} + 214\delta_{x,2} - 784\delta_{x,4} + 2310\delta_{x,5}\right\} . \end{aligned} \tag{5.1.9}$$

Of course, we still have to calculate the sum (5.1.4). Thus, changes of signs in individual orders need not necessarily turn up in the final result. In fact, it turns out that the imaginary part of $C_\Gamma(x)$ is always positive up to order 6 because the smallest orders are positive and they dominate the others. However, for sufficiently small λ the real part does indeed change signs around $x = 4$. We fit (5.1.9) by a complex exponential function:

$$C_\Gamma(x) = a\ e^{\left(\frac{2\pi i}{L} - \frac{1}{\xi_\Gamma}\right)x} + (1-a)\delta_{x,0} \ , \tag{5.1.10a}$$

$$C_\sigma(x) = p\ e^{-\frac{x}{\xi_\sigma}} + q\delta_{x,0} \, . \tag{5.1.10b}$$

[4]) Another natural specialization would be the standard Potts case $\phi = \varphi = 0$. This was discussed in detail in [91]. There, a deviation from the well-known relation (see e.g. [104]) $\xi_\Gamma \sim m(\lambda)^{-1}$ was observed which is clearly due to lattice artifacts.

In (5.1.10) we have also taken into account that from (5.1.8) $\frac{C_\sigma(0)}{C_\sigma(1)} \approx 4$ independent of the correlation length ξ_σ.

If (5.1.10a) is the correct form for $C_\Gamma(x)$ we infer from (5.1.9) that L is about 14 for small λ. We can also see from the higher orders that L increases with increasing λ such that it might well be singular at $\lambda = 1$. The correlation length ξ tends to zero as $\lambda \to 0$. This implies that – after proper re-normalization of the Hamiltonian – the mass gap becomes infinite at $\lambda = 0$. It has already been observed in [68] that there are physical reasons to divide (3.1.1) by $\sqrt{\lambda}$ which would have exactly the effect of infinite mass at $\lambda = 0$. Fits to (5.1.10) for $\lambda \in \{\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\}$ in the superintegrable case are given by the values in table 1.

λ	ξ_Γ	a	L	ξ_σ	p	q	P_{min}	$\frac{LP_{\text{min}}}{2\pi}$
0.25	0.55(3)	0.55(5)	14.3(2)	0.25(2)	0.35(4)	0.32(4)	0.471	1.07(2)
0.50	0.9(1)	0.59(3)	16.5(8)	0.38(4)	0.35(3)	0.24(3)	0.401	1.05(5)
0.75	1.5(6)	0.64(3)	18.3(8)	0.55(6)	0.36(2)	0.09(2)	0.308	0.90(4)

Table 1: Parameters for the correlation functions (5.1.18) at $\phi = \varphi = \frac{\pi}{2}$.

The estimates in table 1 have been obtained as follows. First, ξ_Γ has been estimated by calculating $\mathrm{Re}(\ln(\frac{C_\Gamma(x)}{C_\Gamma(x+1)}))^{-1}$ and averaging over x. Next, the zero of $\mathrm{Re}(e^{\frac{x}{\xi_\Gamma}} C_\Gamma(x))$ has been estimated by linear interpolation for two neighbouring values and $L/4$ was obtained by averaging. Finally, a was estimated such that the difference

$$\mathrm{Re}(C_\Gamma(x)) - a e^{-\frac{x}{\xi_\Gamma}} \cos\left(\frac{2\pi x}{L}\right) \tag{5.1.11}$$

is minimal for $x = 1, 2$. That this procedure yields reasonable fits is demonstrated by Fig. 3 which shows the stretched correlation function $e^{\frac{x}{\xi_\Gamma}} C_\Gamma(x)$ in comparison to the fits. The 'error bars' are not really error bars but given by $a e^{\frac{6-x}{\xi_\Gamma}}$ which gives an idea how much the values have actually been stretched and what might be the contribution of the next orders in the perturbation expansion. The agreement for all x not only in the real part but also in the imaginary part is convincing.

Let us now discuss the implications of (5.1.7) under the assumption that (5.1.10a) is the correct form for general values of the chiral angles. From the leading orders in (5.1.7) we read off the following identity for the ratio of $C_\Gamma(1)$ and $C_\Gamma(2)$:

$$\frac{C_\Gamma(2)}{C_\Gamma(1)} = \frac{\frac{e^{i\frac{2\phi}{3}}}{6\mathcal{C}^2}\lambda^2 + \mathcal{O}(\lambda^3)}{\frac{e^{i\frac{\phi}{3}}}{3\mathcal{C}}\lambda + \mathcal{O}(\lambda^2)} = \frac{e^{i\frac{\phi}{3}}}{2\mathcal{C}}\lambda + \mathcal{O}(\lambda^2). \tag{5.1.12a}$$

On the other hand we immediately obtain from (5.1.10a)

$$\frac{C_\Gamma(2)}{C_\Gamma(1)} = e^{-\frac{1}{\xi_\Gamma}} e^{\frac{2\pi i}{L}}. \tag{5.1.12b}$$

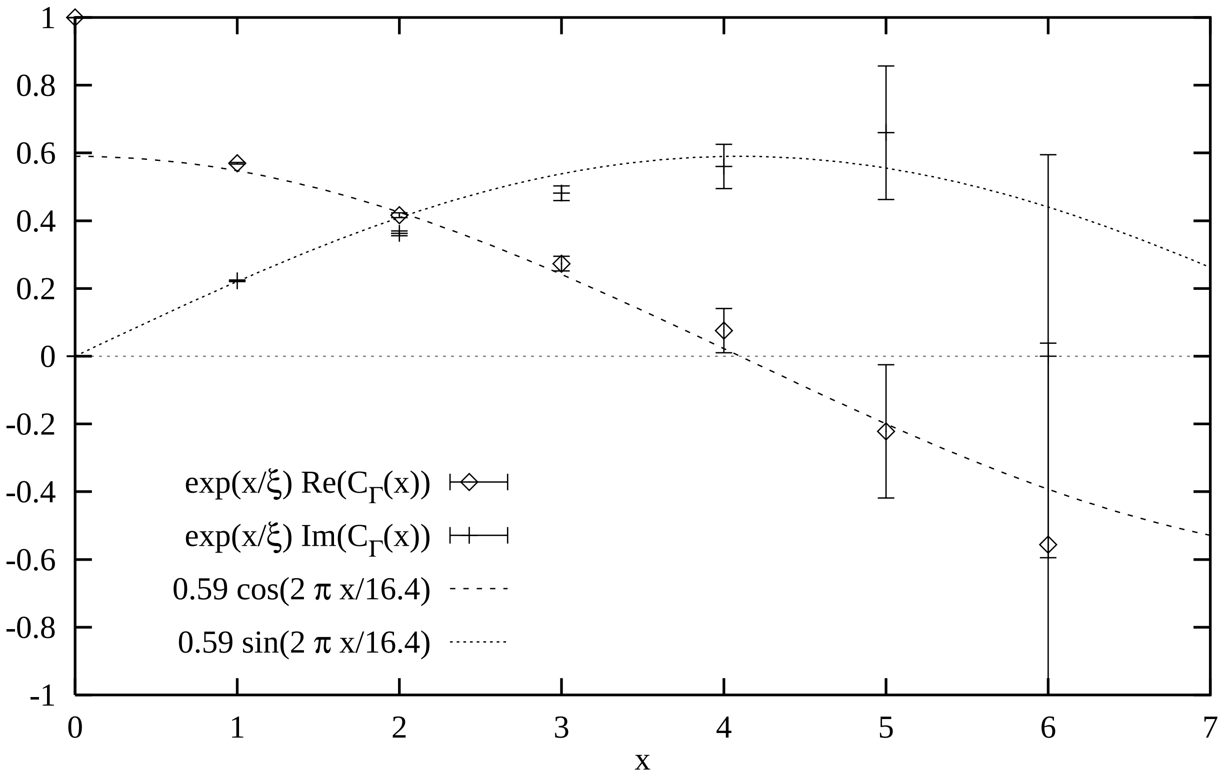

Fig. 3: Correlation function $C_\Gamma(x)$ stretched by $e^{\frac{x}{\xi_\Gamma}}$ in comparison to the fit (5.1.10a) at $\phi = \varphi = \frac{\pi}{2}$, $\lambda = \frac{1}{2}$. The 'error bars' are given by $ae^{\frac{6-x}{\xi_\Gamma}}$ which conveys an idea how much the values have actually been stretched. The oscillatory contribution to $C_\Gamma(x)$ is clearly visible.

Comparison of (5.1.12a) and (5.1.12b) leads to

$$L = \frac{6\pi}{\mathrm{Re}(\phi)} \;, \qquad \xi_\Gamma = -\frac{1}{\ln\left(\frac{\lambda}{2\cos\left(\frac{\varphi}{3}\right)}\right) - \frac{\mathrm{Im}(\phi)}{3}} \tag{5.1.13}$$

for small values of λ. It is noteworthy that we obtain the same result for the oscillation length if we apply a similar argument to $\frac{C_\Gamma(x_1)}{C_\Gamma(x_2)}$ in lowest non-vanishing order with $x_1, x_2 \in \{1,2,3,4\}$. At $\phi = \frac{\pi}{2}$ (5.1.13) yields the approximations $L = 12$, $\xi_\Gamma = 0.52,\ 0.80,\ 1.2$ for $\lambda = 0.25,\ 0.50,\ 0.75$. The agreement with the numbers of table 1 is very good. Thus, for very high temperatures the oscillation length L is proportional to the inverse chiral angle ϕ^{-1}. In particular, the oscillation vanishes smoothly for $\phi \to 0$. According to (4.2.4) for very high temperatures the minimum of the dispersion relation of the fundamental particles is also proportional to ϕ – for $n = 3$ and $Q = 1$ we have $P_{\min} = \frac{\mathrm{Re}(\phi)}{3}$. Thus, we obtain from (5.1.13) for very high temperatures

$$P_{\min} L \mid_{\lambda \to 0} = 2\pi \qquad \forall \phi, \varphi. \tag{5.1.14}$$

Furthermore, the second order in (4.2.7) shows that the minimal momentum $P_{\min}$ decreases with increasing λ (compare also [69]). Similarly, we read off from (5.1.7) that the inverse oscillation length L^{-1} also decreases with increasing inverse temperature λ. Thus, (5.1.14) has a chance to be valid for all values of λ in the massive high-temperature phase. Indeed, using the values of $P_{\min}$ given in table 8 of [68] we see that $P_{\min}L = 2\pi$ holds quite accurately for $\lambda = 0.25, 0.5, 0.75$ at $\phi = \varphi = \frac{\pi}{2}$ (compare table 1). We suspect that in general this relation is not exact but an excellent approximation.

Note that even at $\phi = \varphi = \frac{\pi}{2}$ the correlation lengths ξ_Γ and ξ_σ are clearly different. Furthermore, ξ_σ coincides with its dual in the low-temperature phase whereas ξ_Γ does not (see [82]). This can be understood in terms of the form factor decomposition to be presented in section 5.4 (see [91]).

5.2. Numerical computation of the correlation functions

In this section we study the correlation function for the operator Γ of the $\mathbb{Z}_3$-chain numerically. We will in particular check the relation (5.1.14) numerically.

In order to evaluate the correlation function (5.1.5) numerically one needs the groundstate of the Hamiltonian (3.1.1). The groundstate of the $\mathbb{Z}_3$-chain is easily obtained for general values of the parameters (even in the non-hermitian case $\phi \in \mathbb{C}$) using vector iteration up to $N = 13$ sites. The more difficult point is to calculate the matrix elements of $\Gamma^+_{x+1}\Gamma_1$ because this operator does not conserve momentum and thus does not leave a space of momentum eigenstates invariant. It is crucial to really work with $\Gamma^+_{x+1}\Gamma_1$ and *not* to replace it by $\frac{1}{N}\sum_{r=1}^{N}\Gamma^+_{x+r}\Gamma_r$ because this would destroy the oscillation. Table 2 shows the correlation function $C_\Gamma(x)$ obtained in this manner for $N = 12$ and $N = 13$ sites at $\phi = \varphi = \frac{\pi}{2}$, $\lambda = \frac{1}{2}$ which corresponds to Fig. 3. This table also contains the perturbative results for the correlation function $C_\Gamma^{\mathrm{pert.}}(x)$ which were obtained in section 5.1.

x	0	1	2	3	4	5	6
$C_\Gamma^{\mathrm{pert.}}(x)$	1	$.18868+.07384i$	$.04561+.03980i$	$.00992+.01747i$	$.00091+.00674i$	$-.00088+.00263i$	$-.00074$
$C_\Gamma^{12,\mathrm{num.}}(x)$	1	$.18881+.07385i$	$.04587+.03967i$	$.01004+.01737i$	$.00126+.00679i$	$-.00056+.00224i$	$-.00080$
$C_\Gamma^{13,\mathrm{num.}}(x)$	1	$.18882+.07385i$	$.04588+.03967i$	$.01007+.01738i$	$.00132+.00684i$	$-.00043+.00242i$	$-.00063+.00058i$

Table 2: Perturbative results and numerical results for $N = 12$ and $N = 13$ sites for the correlation function $C_\Gamma(x)$ at $\phi = \varphi = \frac{\pi}{2}$, $\lambda = \frac{1}{2}$.

The agreement between the results of both methods and also between $N = 12$ and $N = 13$ sites is good. This shows that on the one hand higher orders are indeed negligible in (5.1.9) for $x < 7$ and on the other hand that the finite chain length does not considerably affect the correlation function $C_\Gamma(x)$. Thus, one can take the values obtained e.g. at $N = 12$ sites as an approximation for the infinite chain limit as long as $x \leq 6$.

Table 3 collects results of numerical calculations at $N = 12$ sites for the self-dual values $\phi = \varphi \in \{\frac{3\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{8}\}$ and a few integrable cases.

φ	ϕ	λ	ξ_Γ	L	a	P_{min}	$\frac{LP_{\text{min}}}{2\pi}$
$\frac{3\pi}{4}$	$\frac{3\pi}{4}$	$\frac{1}{4}$	0.62(8)	10(1)	0.4(2)	0.746	1.18 ± 0.12
$\frac{3\pi}{4}$	$\frac{3\pi}{4}$	$\frac{1}{2}$	1.2(6)	12(1)	0.4(1)	$0.685^\dagger$	1.34 ± 0.14
$\frac{3\pi}{4}$	$\frac{3\pi}{4}$	$\frac{3}{4}$	1.4(1)	16(1)	0.65(3)	$0.602^\dagger$	1.54(8)
$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\frac{1}{4}$	0.6(1)	14.05(6)	0.44(8)	0.470	1.051(4)
$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\frac{1}{2}$	0.60(5)	16(1)	0.59(3)	0.401	1.07(8)
$\frac{\pi}{2}$	$\frac{\pi}{2}$	$\frac{3}{4}$	1.3(2)	29(6)*		0.189	0.9(2)
$\frac{3\pi}{8}$	$\frac{3\pi}{8}$	$\frac{1}{4}$	0.53(3)	18(2)	0.62(1)	0.341	1.0(1)
$\frac{3\pi}{8}$	$\frac{3\pi}{8}$	$\frac{1}{2}$	0.8(2)	25(1)*		0.283	1.14(6)
$\frac{3\pi}{8}$	$\frac{3\pi}{8}$	$\frac{3}{4}$	1.8(6)	50 ± 23*		0.211	1.7(8)
$\frac{3\pi}{8}$	$-i\,0.98942$	$\frac{1}{4}$	0.7(2)	∞		0	
$\frac{3\pi}{8}$	0.69919	$\frac{1}{2}$	1.1(3)	49(7)*		0.159	1.2(2)
$\frac{3\pi}{4}$	$\pi + i\,1.70004$	$\frac{1}{4}$	1.0(5)	5.9(1)	0.3(1)	$\frac{\pi}{3}$	0.99(2)

Table 3: Parameters for the correlation function (5.1.10a) calculated numerically for $N = 12$ sites.

The real part of the correlation function C_Γ has no zero in the interval [0,6] for the entries marked with a '*'. Therefore, the procedure of section 5.1 could not be used for the computation of L. Here L has instead been obtained by the formula

$$L = \frac{1}{4} \sum_{x=1}^{4} \frac{2\pi}{\text{Im}\left(\ln\left(\frac{C_\Gamma(x)}{C_\Gamma(x+1)}\right)\right)} . \tag{5.2.1}$$

The values of P_{min} in table 3 have been obtained by first calculating $\mathsf{E}_1(P)$ numerically at $N = 12$ sites and afterwards minimizing the finite fourier decomposition of $(\mathsf{E}_1(P))^2$ numerically. This method for estimating P_{min} failed for those values marked with a '$\dagger$' because here $\mathsf{E}_1(P)$ partly crosses two-particle scattering states. $\mathsf{E}_1(P)$ becomes even negative for $\phi = \varphi = \frac{3\pi}{4}$, $\lambda = \frac{3}{4}$. This implies that the groundstate does not belong to the $Q = P = 0$ sector and this point in the parameter space lies in the massless incommensurate phase. However, we have ignored this fact and used the lowest energy state in the $Q = P = 0$ sector for evaluation of the correlation functions. This is justified because it yields results that are similar to those for the other values of the parameters. The values of P_{min} marked with a '$\dagger$' have been determined by first determining the smallest energy gap in the $Q = 1$ sector at *finite* $N = 8, \ldots, 12$. For $8 \leq N \leq 12$ the minimum of the discretized dispersion relation is located at $P = \frac{2\pi}{N}$. Next, a polynomial interpolation between these five values for the energy gap was minimized numerically.

That the above procedures yield reasonable fits was demonstrated by a figure in [69].

We have also included a few values for integrable points at the end of table 3, i.e. points where the parameters satisfy $\cos\varphi = \lambda \cos\phi$. For $\varphi = \frac{3\pi}{8}$, $\lambda = \frac{1}{2}$, the integrable case is hermitean and behaves precisely like the self-dual case $\phi = \varphi$. For small values of λ one has to choose one of the angles φ, ϕ complex in order to satisfy the integrability-condition (3.1.13). We choose ϕ complex: For $\varphi < \frac{\pi}{2}$ we choose purely complex $\phi \in i\mathbb{R}$ whereas for $\varphi > \frac{\pi}{2}$ we take $\phi - \pi \in i\mathbb{R}$ (compare also [126]). For complex choices of ϕ the Hamiltonian becomes non-hermitean such that the excitation energies become complex. Thus, $P_{\min}$ is not strictly the minimum of the dispersion relations but instead a point of symmetry – compare [126, 91, 69] and in particular section 5.4 below.

The agreement with the prediction $LP_{\min} = 2\pi$ is good for all values in table 3 bearing in mind that we have ignored systematic errors. This applies also to the point $\phi = \varphi = \frac{3\pi}{4}$, $\lambda = \frac{3}{4}$ in the massless incommensurate phase because here the estimate for the error of L is probably too small.

5.3. Correlation functions in the low-temperature regime

In this section we apply the method explained in section 5.1 to the correlation functions in the low-temperature phase of the $\mathbb{Z}_3$-chiral Potts quantum chain. Note that the duality argument of section 3.2 applies only to the Hamiltonian and not to other operators. Thus, quantities like e.g. correlation lengths may be different in these two phases.

We study again the correlation functions $C_\Gamma(x)$ and $C_\sigma(x)$ as defined by (5.1.2) and (5.1.5) using a low-temperature expansion for the ground state from the state $|\,\mathrm{GS}\rangle^{\,Q}$ (3.2.2). The expansion of the ground state in powers of $\tilde{\lambda}$ leads to an expansion of the correlation functions in powers of $\tilde{\lambda}$:

$$C_\Xi(x) = \sum_{k=0}^{\infty} \tilde{\lambda}^k \tilde{C}_\Xi^{(k)}(x). \tag{5.3.1}$$

Below, we will first give the final results for general angles ϕ, φ. We then specialize to the superintegrable case $\phi = \varphi = \frac{\pi}{2}$ and calculate even higher orders. By looking for a good fit we try to guess the structure of the correlation functions – as before. With this experience we turn back to the general case and discuss how the correlation functions should change for general ϕ, φ.

In order to save space we present only the final results for the correlation functions. For $C_\Gamma(x)$ one obtains, using the abbreviations $\tilde{\mathcal{C}} = \cos\left(\frac{\phi}{3}\right)$, $\tilde{\mathcal{R}} = 1 - 4\tilde{\mathcal{C}}^2$:

$$\begin{aligned}
&\tilde{C}_\Gamma^{(0)}(x) = 1 \ , && \tilde{C}_\Gamma^{(1)}(x) = 0 \ , \\
&\tilde{C}_\Gamma^{(2)}(x) = \frac{1}{6\tilde{\mathcal{C}}^2}\left\{\delta_{x,0} - 1\right\} \ , && \tilde{C}_\Gamma^{(3)}(x) = \frac{\cos\varphi}{18\tilde{\mathcal{C}}^3}\left\{\delta_{x,0} - 1\right\} \ , \\
&\tilde{C}_\Gamma^{(4)}(x) = &&
\end{aligned}$$

$$\frac{1}{27\tilde{\mathcal{C}}^2}\left\{(1-\delta_{x,0})\left(\frac{2(1-16\tilde{\mathcal{C}}^2)}{3\tilde{\mathcal{R}}^2} + \frac{1}{16\tilde{\mathcal{C}}^2}\right) + \delta_{x,1}\left(\frac{1+2\tilde{\mathcal{C}}^2 - 3\ i\ \sin\left(\frac{2\phi}{3}\right)}{3\tilde{\mathcal{R}}^2} + \frac{5}{16\tilde{\mathcal{C}}^2}\right)\right\}. \tag{5.3.2}$$

The first orders of the correlation function $C_\sigma(x)$ read as follows:

$$\begin{aligned}
&\tilde{C}_\sigma^{(0)}(x) = \delta_{x,0} \ , && \tilde{C}_\sigma^{(1)}(x) = 0 \ , \\
&\tilde{C}_\sigma^{(2)}(x) = -\frac{1}{9}\left\{\frac{\delta_{x,0}}{\tilde{\mathcal{C}}^2} + \delta_{x,1}\left(\frac{2}{\tilde{\mathcal{R}}} + \frac{1}{2\tilde{\mathcal{C}}^2}\right)\right\} \ , && \tilde{C}_\sigma^{(3)}(x) = -\frac{\cos\varphi}{9\tilde{\mathcal{C}}}\left\{\frac{\delta_{x,0}}{2\tilde{\mathcal{C}}^2} + \frac{\delta_{x,1}}{\tilde{\mathcal{R}}}\right\} \ , \\
&\tilde{C}_\sigma^{(4)}(x) =
\end{aligned}$$

$$\frac{1}{81\tilde{\mathcal{C}}^2}\left\{\delta_{x,0}\left(\frac{7}{16\tilde{\mathcal{C}}^2} + \frac{8}{\tilde{\mathcal{R}}}\right) + \delta_{x,1}\left(\frac{15}{16\tilde{\mathcal{C}}^2} + \frac{29}{12\tilde{\mathcal{R}}} - \frac{16\tilde{\mathcal{C}}^4}{\tilde{\mathcal{R}}^3}\right) + \delta_{x,2}\left(-\frac{1}{8\tilde{\mathcal{C}}^2} + \frac{7+44\tilde{\mathcal{C}}^2}{12\tilde{\mathcal{R}}^2}\right)\right\}. \tag{5.3.3}$$

Note that the correlation functions (5.3.2) and (5.3.3) do not depend on the charge sector.

Eq. (5.3.2) suggests that the correlation function $C_\Gamma(x)$ tends to a non-zero constant for large distances x – in contrast to the correlation functions in the high-temperature phase so that that the low-temperature phase is ordered over long ranges. However, beyond this general conclusion, it is difficult to guess from (5.3.2) or (5.3.3) what might be the behaviour even for small x. Thus, we set $\phi = \varphi = \frac{\pi}{2}$, calculate four further orders and obtain

$$\begin{aligned}
&\tilde{C}_\Gamma^{(0)}(x) = 1 \ , \qquad \tilde{C}_\Gamma^{(1)}(x) = \tilde{C}_\Gamma^{(3)}(x) = \tilde{C}_\Gamma^{(5)}(x) = \tilde{C}_\Gamma^{(7)}(x) = 0 \ , \\
&\tilde{C}_\Gamma^{(2)}(x) = \frac{2}{9}\left(\delta_{x,0} - 1\right) \ , \\
&\tilde{C}_\Gamma^{(4)}(x) = \frac{7}{81}\left(\delta_{x,0} - 1\right) + \delta_{x,1}\frac{5 - i\sqrt{3}}{162} \ , \\
&\tilde{C}_\Gamma^{(6)}(x) = \frac{1}{6561}\left\{336\left(\delta_{x,0} - 1\right) + 160\delta_{x,1} + 60\delta_{x,2}\right\} - i\frac{\sqrt{3}}{6561}\left\{26\delta_{x,1} + 20\delta_{x,2}\right\} \ , \\
&\tilde{C}_\Gamma^{(8)}(x) = \frac{1}{354294}\left\{12600\left(\delta_{x,0} - 1\right) + 6852\delta_{x,1} + 3521\delta_{x,2} + 1225\delta_{x,3}\right\} \\
&\qquad\qquad - i\frac{\sqrt{3}}{354294}\left\{960\delta_{x,1} + 995\delta_{x,2} + 525\delta_{x,3}\right\}
\end{aligned} \tag{5.3.4}$$

and

$$\begin{aligned}
&\tilde{C}_\sigma^{(0)}(x) = \delta_{x,0} \ , \qquad \tilde{C}_\sigma^{(1)}(x) = \tilde{C}_\sigma^{(3)}(x) = \tilde{C}_\sigma^{(5)}(x) = \tilde{C}_\sigma^{(7)}(x) = 0 \ , \\
&\tilde{C}_\sigma^{(2)}(x) = \frac{1}{27}\left\{-4\delta_{x,0} + \delta_{x,1}\right\} \ , \\
&\tilde{C}_\sigma^{(4)}(x) = \frac{1}{729}\left\{-41\delta_{x,0} + 14\delta_{x,1} + 8\delta_{x,2}\right\} \ , \\
&\tilde{C}_\sigma^{(6)}(x) = \frac{1}{19683}\left\{-586\delta_{x,0} + 147\delta_{x,1} + 126\delta_{x,2} + 80\delta_{x,3}\right\} \ , \\
&\tilde{C}_\sigma^{(8)}(x) = \frac{1}{531441}\left\{-9927\delta_{x,0} + 2130\delta_{x,1} + 1721\delta_{x,2} + 1728\delta_{x,3} + 910\delta_{x,4}\right\}.
\end{aligned} \tag{5.3.5}$$

Up to the order calculated, $C_\sigma(x)$ is real for all values of the parameters ϕ, φ, $\tilde{\lambda}$. $C_\Gamma(x)$, in contrast, has a non-vanishing imaginary part. By analogy to the high-temperature regime and from the results in [105, 66] we expect that $C_\Gamma(x)$ is oscillating. Indeed, the correlation functions in the superintegrable case $\phi = \varphi = \frac{\pi}{2}$ can nicely be fitted by

$$C_\sigma(x) = a\delta_{x,0} + be^{-\frac{x}{\xi_\sigma}} \ , \tag{5.3.6a}$$

$$C_\Gamma(x) = m^2 + pe^{-\left(\frac{1}{\xi_\Gamma}+\frac{2\pi i}{L}\right)x}. \tag{5.3.6b}$$

For $\tilde{\lambda} \in \left\{\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right\}$ good fits to (5.3.4) and (5.3.5) using (5.3.6) are given by the values in table 4.

$\tilde{\lambda}$	ξ_σ	a	b	ξ_Γ	m^2	L	p	$\xi_\Gamma^{\text{num.}}$	$L^{\text{num.}}$
0.25	0.26(1)	0.891(9)	0.099(9)	0.24(3)	0.9857605	30 ± 18	0.011(3)	0.26(3)	27 ± 7
0.50	0.41(2)	0.841(7)	0.118(7)	0.37(5)	0.9381	30 ± 15	0.05(1)	0.42(6)	30 ± 8
0.75	0.58(5)	0.74(1)	0.16(1)	0.50(7)	0.832	30 ± 13	0.15(2)	0.6(1)	28 ± 4

Table 4: Parameters for the correlation functions (5.3.6) at $\phi = \varphi = \frac{\pi}{2}$.

First, we remark that the correlation lengths satisfy $\xi_\sigma = \xi_\Gamma =: \xi$ for all values of $\tilde{\lambda}$ within the numerical accuracy. In fact, one expects this equality because the correlation lengths should be the inverses of some mass scale, and there is only one mass scale in our problem because all three charge sectors are degenerate. Furthermore, we observe that our data is compatible with an oscillating correlation function for the operator Γ. The oscillation length L (or wave vector) is around 30 sites in a major part of the low-temperature phase. In [105, 66] it has been predicted that L should diverge as $\tilde{\lambda}$ crosses the phase boundary and approaches $\tilde{\lambda} = 1$ where the critical exponent is expected to equal $\frac{2}{3}$. Our results are compatible with a divergent oscillation length at $\tilde{\lambda} = 1$ although due to the large errors we do not even see that L increases with $\tilde{\lambda}$.

In addition to the perturbation expansions we can also perform numerical evaluations of the correlation function $C_\Gamma(x)$. Since we can use vector iteration for up to $N = 13$ sites implying a distance of up to $x = 6$ one might hope to obtain more accurate results with this method. That this is not really the case is demonstrated by the values $\xi_\Gamma^{\text{num.}}$ and $L^{\text{num.}}$ which we have included into table 4. The main problem with numerical calculations is the numerical accuracy: In particular, the evaluation of the constant contribution m^2 is not free of errors. On the other hand the short correlation lengths strongly damp the non-constant part of the correlation functions: For example $C_\Gamma(x) - m^2$ has already decreased by 10 orders of magnitude at $x = 6$ for $\tilde{\lambda} = \frac{1}{4}$. Therefore, for our estimates we have used only $x \leq 4$ for $\tilde{\lambda} = \frac{1}{4}$ and $x \leq 5$ for $\tilde{\lambda} = \frac{1}{2}$ and $\tilde{\lambda} = \frac{3}{4}$.
Thus, it will be very difficult to obtain more precise results from approximative arguments and an exact expression for $C_\Gamma(x)$ is probably needed in order to decide whether (5.3.6b) really is the correct form and to determine the wave vector L accurately.

Before we conclude the discussion of the correlation functions for the superintegrable chiral Potts model, we mention that a conjecture for the form of $C_\Gamma(x)$ has been formulated in [4]: $C_\Gamma(x) = m^2 + \mathcal{O}(e^{-\frac{x}{\xi_\Gamma}})$ where m is the order parameter. Our result (5.3.6) is compatible with this from. In [97] the conjecture for the order parameter

$$m = \frac{\langle \tilde{v} \mid \Gamma_x \mid \tilde{v} \rangle}{\langle \tilde{v} \mid \tilde{v} \rangle} = \left(1 - \tilde{\lambda}^2\right)^{\frac{1}{9}} \tag{5.3.7}$$

has been formulated, but (5.3.7) has not been proven yet. The constant term in (5.3.4) is in exact agreement with (5.3.6) and (5.3.7) up to the order calculated, such that we may assume that at least the constant term of $C_\Gamma(x)$ is now known exactly.

A few remarks on the choice of ground state (3.2.2) are in place because in [97, 11] (5.3.7) has actually been derived considering an expectation value of the operator Γ_x. We have already pointed out that the one point functions of Γ_x vanish identically due to charge conservation if one uses the charge eigenstates (3.2.2). However, if one uses instead non-charge eigenstates like $|\,0\ldots 0\rangle$ for a perturbative expansion of $|\,\tilde{v}\rangle$ they do not vanish. Indeed, using an expansion for $|\,\tilde{v}\rangle$ from $|\,0\ldots 0\rangle$ we once again verified equality of this one point function with the order parameter m. If we redefine $\bar{C}_\Gamma(x)$ by replacing $|\,v\rangle$ by $|\,\tilde{v}\rangle$ and subtracting the contribution from the one point functions, this is in fact the only change, i.e. $\bar{C}_\Gamma(x) = C_\Gamma(x) - m^2$. $C_\sigma(x)$ remains unchanged under this redefinition.

For more general values of the angles ϕ, φ one expects the correlation functions to be also of the form (5.3.6) – of course with different values of the parameters. We can see from the constant term m^2 of the correlation function $C_\Gamma(x)$ (5.3.2) that it will not be of the form (5.3.7) for general $\phi \neq \frac{\pi}{2} \neq \varphi$. In general, the coefficient of $\tilde{\lambda}^3$ for the constant term does not vanish and m^2 does not even have an expansion in powers of $\tilde{\lambda}^2$. Among the powers that we have calculated for the general case only the fourth order in (5.3.2) has a non-vanishing imaginary part at $x = 1$. Under the assumption that (5.3.6b) is the general form we would expect the imaginary part at $x = 1$ to be proportional to $\sin\left(\frac{2\pi}{L}\right)$ for very small temperatures $\tilde{\lambda}$. Thus, we expect for very low temperatures $\tilde{\lambda}$ the relation $L^{-1} \sim \phi$. On the one hand, this explains the conjectured presence of a second length scale L in addition to the correlation length ξ. The oscillation length L just comes from the chiral angle ϕ and thus these two scales must be related to each other. On the other hand, the oscillation (should it really be present) will vanish smoothly as the parity conserving Potts case $\phi = \varphi = 0$ is approached.

5.4. Form factors and correlation functions

In this section we show how to use form factors in order to determine the oscillation length L exactly using symmetries of the Hamiltonian arising for particular values of the parameters.

One can use the quasiparticle picture which we have discussed earlier in order to rewrite a correlation function $C_\Xi(x)$ as follows:

$$\begin{aligned} C_\Xi(x) &= \frac{\sum_{n=0}^{\infty} \int_0^{2\pi} \left(\prod_{i=1}^n \mathrm{d}p_i\right) \langle v \,|\; \Xi_{x+1}^{+} \,|\, p_1, \ldots, p_n \rangle \langle p_1, \ldots, p_n \,|\; \Xi_1 \;|\, v \rangle}{\langle v \,|\, v \rangle} - \frac{|\langle v \,|\; \Xi_1 \;|\, v \rangle\,|^2}{\langle v \,|\, v \rangle^{\,2}} \\ &= \sum_{n=1}^{\infty} \int_0^{2\pi} \left(\prod_{i=1}^{n} \mathrm{d}p_i\right) \; e^{ix\left(\left(\sum_{j=1}^n p_j\right) - P_{|v\rangle}\right)} \; \frac{|\langle p_1, \ldots, p_n \,|\; \Xi_1 \;|\, v \rangle\,|^2}{\langle v \,|\, v \rangle} \end{aligned} \tag{5.4.1}$$

where we have inserted a complete set of normalized n-particle states $|\, p_1, \ldots, p_n \rangle$. Representations similar to (5.4.1) have been used in quantum field theory for a long time (see e.g. [107]) and are well-known to be useful for the evaluation of correlation functions of statistical models (see e.g. [111]). According to (5.4.1) one could compute the correlation function $C_\Xi(x)$ by computing its '*form factors*' $\langle p_1, \ldots, p_n \mid \Xi_1 \mid v \rangle$, but one can even derive interesting results without doing so. Clearly, if the groundstate $|\, v\rangle$ has non-zero momentum $P_{|v\rangle} \neq 0$ we expect an oscillatory contribution to the correlation function. However, one can read off from (5.4.1) that an oscillatory contribution is also to be expected if $P_{|v\rangle} = 0$ but the model breaks parity which precisely applies to the massive high-temperature phase of the chiral Potts model. The correlation functions of massive models in general have an exponential decay, i.e. $C_\Xi(x) = e^{-\frac{x}{\xi}} f_\Xi(x)$ where $f_\Xi(x)$ is some bounded function. According to (5.4.1) we also expect an oscillatory contribution of the form $e^{i\frac{2\pi x}{L}}$. In summary, we expect correlation functions of the approximate form

$$C_\Xi(x) \sim e^{-\frac{x}{\xi}+i\frac{2\pi x}{L}}. \tag{5.4.2}$$

ξ is called 'correlation length' and L is the 'oscillation length' (L^{-1} is the 'wave vector'). Eq. (5.4.2) explains the fits (5.1.10) and (5.3.6) that we have used earlier. More precisely, for the $\mathbb{Z}_n$-chiral Potts model the operator Γ_1 creates $Q = 1$-single-particle excitations from the groundstate. The dispersion relations of these particles clearly violate parity. Therefore we expect that $C_\Gamma(x)$ is of the form (5.4.2). The action of the operator σ_1 is much less spectacular. In particular, it leaves the charge sector $Q = 0$ invariant and thus it need not necessarily have an oscillatory contribution. In fact, from (5.1.3) we see that $C_\sigma(x)$ should be real which in view of (5.4.2) implies the absence of oscillations.

For massive perturbations of conformal field theories it is well-known that form factor expansions already for few particles yield excellent approximations (see e.g. [111]). In order to gain some intuition we perform some simple computations for the form factors of the operator Γ for the $\mathbb{Z}_3$-chain.

First, considering perturbation series for the states one sees that

$$\langle p_1, \ldots, p_r \mid \Gamma_1 \mid v\rangle = \mathcal{O}(\lambda^{[\frac{r}{2}]}). \tag{5.4.3}$$

Next we compute the states $|\, v\rangle$ and $|\, p_1\rangle$ from perturbation series of (4.2.1) and (4.2.2) respectively. One finds that up to order λ the states are already normalized properly, i.e.

$$\langle v \,|\, v\rangle = 1 + \mathcal{O}(\lambda^2), \qquad \langle p_1 \,|\, p_1\rangle = 1 + \mathcal{O}(\lambda^2). \tag{5.4.4}$$

Finally one finds the single-particle form factor for $n = 3$ up to order λ:

$$\langle p_1 \mid \Gamma_1 \mid v\rangle = \frac{1}{\sqrt{\int 1 \mathrm{d}p}} \left\{ 1 + \lambda \frac{\cos\left(p_1 - \frac{\phi}{3}\right)}{3\cos\left(\frac{\varphi}{3}\right)} + \mathcal{O}(\lambda^2) \right\}. \tag{5.4.5}$$

Comparing (5.4.5) with (4.2.7) up to order λ one sees that the maximum of the form factor is obtained when $\mathsf{E}_1(p_1)$ has a minimum and vice versa. Furthermore, multi-particle states have higher energy than single-particle states and due to (5.4.3) the contributions of the form factors decrease with the number of particles for small λ. In summary, one obtains the qualitative statement that the contributions of the form factors decrease with increasing energy.

According to (5.4.3) the single-particle form factor (5.4.5) is the only one contributing to $C_\Gamma(x)$ up to order λ. Indeed upon inserting (5.4.5) into (5.4.1) one recovers (5.1.7) up to first order in λ – as it should be. Note however that the direct computation of (5.1.7) is simpler than the one using a form factor expansion.

Symmetries of the Hamiltonian translate into symmetries of the form factors. In certain cases these symmetries are already sufficient to compute the oscillation length L as we will see now.

Def. VI: (Parity operator) The parity operator $\mathfrak{P}$ is defined by the following action on the states (3.1.6):

$$r(\mathfrak{P})\,|i_1\ldots\ldots i_N\rangle = |i_1 i_N i_{N-1}\ldots\ldots i_2\rangle\,. \tag{5.4.6}$$

Remark: $\mathfrak{P}\sigma_{1+x}\mathfrak{P} = \sigma_{1-x}$, $\mathfrak{P}\Gamma_{1+x}\mathfrak{P} = \Gamma_{1-x}$.

The following lemma is based on results obtained via numerical diagonalization in [126] which showed that the Hamiltonian (3.1.1) has exact symmetries for particular values of the parameters:

Lemma I: *Denote the restriction of the Hamiltonian $H_N^{(n)}$ in eq. (3.1.1) to the spaces with momentum P and charge Q by '$H_N^{(n)}(P,Q)$'. Then one has the following identities (see also [126]):*

$$\begin{aligned}
\alpha_k = \alpha_{n-k} \quad &\Rightarrow \quad \mathfrak{P}H_N^{(n)}(P,Q)\mathfrak{P} = H_N^{(n)}(-P,Q)\,,\\
\bar{\alpha}_k^* = \bar{\alpha}_{n-k} \text{ and } \alpha_k \in \mathbb{R} \quad &\Rightarrow \quad \mathfrak{P}H_N^{(n)}(P,Q)\mathfrak{P} = \Big(H_N^{(n)}(-P,Q)\Big)^+\,,\\
\bar{\alpha}_k^* = \bar{\alpha}_{n-k} \text{ and } \alpha_k^* = e^{-2\pi i z k}\alpha_k \quad &\Rightarrow \quad \mathfrak{P}H_N^{(n)}(P_{\mathrm{m},Q}+P,Q)\mathfrak{P} = \Big(H_N^{(n)}(P_{\mathrm{m},Q}-P,Q)\Big)^+
\end{aligned} \tag{5.4.7}$$

where the symmetry of the last line holds for any Q that is invertible in $\mathbb{Z}_n$ and those $P_{\mathrm{m},Q}$ satisfying $P_{\mathrm{m},Q}Q^{-1} + \pi z \equiv 0$ mod π as well as $e^{i2P_{\mathrm{m},Q}}$ being an nth root of unity. For very particular values of the momentum P and the chain length N some projection is necessary in (5.4.7). ■

The first two lines of (5.4.7) follow immediately by looking at $\mathfrak{P}H_N^{(n)}\mathfrak{P}$, keeping in mind that the translation operator defined in (3.1.10) satisfies $\mathfrak{P}T_N\mathfrak{P} = T_N^{-1} = T_N^+$. The derivation of the third line of (5.4.7) is more complicated and relies on a suitable choice of basis. Because of its technicality we have shifted it to appendix B.

Remarks:

1) For the last line of (5.4.7) insert the parameterization (3.1.12) and set $z = \frac{2}{n}$. Then $P_{\mathrm{m},Q} = \pi(1 - \frac{2Q}{n})$ is a solution to $P_{\mathrm{m},Q}Q^{-1} + \frac{2\pi}{n} = 0$ lying in the interval $[-\pi,\pi]$ – the other solution is shifted by π. The solution $P_{\mathrm{m},Q} = \pi(1 - \frac{2Q}{n})$ corresponds to the minimum (4.2.4) of the dispersion relation of the single-particle state in this charge sector.
2) The restriction to Q invertible in $\mathbb{Z}_n$ (those Q whose greatest common divisor with n is 1) was necessary for technical reasons but there are indications that lemma I is

true without this restriction. Combining this with remark 1) we conclude that the relation $P_{\mathrm{m},Q} = \pi(1 - \frac{2Q}{n})$ seems to be valid for general Q. In fact, close inspection of the argument in appendix B shows that the assumptions can be weakened in order to cover e.g. also the case $Q = 2$ for $n = 4$.

3) In the generic case (which is the only case we are really interested in) one may ignore the projection operators in the equality (5.4.7).

Theorem VI: *(Oscillation length [91]) Let the Hamiltonian $H(P,Q)$ restricted to momentum and charge eigenspaces with eigenvalues P and Q have one of the following symmetries:*

$$\mathfrak{P} H(P_{\mathrm{m},Q}{+}P,Q)\mathfrak{P} = H(P_{\mathrm{m},Q}{-}P,Q) \qquad \text{or} \qquad \mathfrak{P} H(P_{\mathrm{m},Q}{+}P,Q)\mathfrak{P} = \left(H(P_{\mathrm{m},Q}-P,Q)\right)^{+} \tag{5.4.8}$$

with some $P_{\mathrm{m},Q}$ depending on the charge sector Q. Assume furthermore that $P_{|v\rangle} = 0$ and that $\Xi_1\,|v\rangle$ has charge Q. Then the oscillation length L of the correlation function $C_\Xi(x)$ satisfies

$$L P_{\mathrm{m},Q} = 2\pi\,. \tag{5.4.9}$$

■

Proof: We start from the form factor expansion (5.4.1) which in the present case becomes

$$C_\Xi(x) = \sum_r \int_0^{2\pi} \mathrm{d}P\, e^{iPx}\, \frac{|\langle P,Q;r\,|\,\Xi_1\,|v\rangle\,|^2}{\langle v\,|\,v\rangle} \tag{5.4.10}$$

where we have only written the quantum numbers P and Q explicitly and comprised the other ones in the label 'r'. First we observe that $\mathfrak{P}\Xi_1\mathfrak{P} = \Xi_1$. If the Hamiltonian satisfies $\mathfrak{P} H(P_{\mathrm{m},Q}{+}P,Q)\mathfrak{P} = H(P_{\mathrm{m},Q}{-}P,Q)$, then eigenstates of momentum $P_{\mathrm{m},Q}{+}P$ are mapped under parity to eigenstates of momentum $P_{\mathrm{m},Q}{-}P$. This means that $\langle (P_{\mathrm{m},Q}{+}P),Q;r\,|\,\Xi_1\,|v\rangle = \langle (P_{\mathrm{m},Q}-P),Q;r\,|\,\Xi_1\,|v\rangle$. If the symmetry involves the adjoint of the Hamiltonian one finds $\langle (P_{\mathrm{m},Q}+P),Q;r\,|\,\Xi_1\,|v\rangle = \langle (P_{\mathrm{m},Q}-P),Q;r\,|\,\Xi_1\,|v\rangle^*$. Thus, the following identity is valid in both cases:

$$|\langle (P_{\mathrm{m},Q}+P),Q;r\,|\,\Xi_1\,|v\rangle\,|^2 = |\langle (P_{\mathrm{m},Q}-P),Q;r\,|\,\Xi_1\,|v\rangle\,|^2\,. \tag{5.4.11}$$

Now we turn back to the form factor expansion (5.4.10):

$$\begin{aligned}
C_\Xi(x) &= \sum_r \left\{ \int\limits_{P_{\mathrm{m},Q}}^{P_{\mathrm{m},Q}+\pi} \mathrm{d}P\, e^{iPx}\, \frac{|\langle P,Q;r\,|\,\Xi_1\,|v\rangle\,|^2}{\langle v\,|\,v\rangle} + \int\limits_{P_{\mathrm{m},Q}-\pi}^{P_{\mathrm{m},Q}} \mathrm{d}P\, e^{iPx}\, \frac{|\langle P,Q;r\,|\,\Xi_1\,|v\rangle\,|^2}{\langle v\,|\,v\rangle} \right\} \\
&= \sum_r \int\limits_0^{\pi} \mathrm{d}P\, \left\{ e^{i(P_{\mathrm{m},Q}+P)x}\, \frac{|\langle (P_{\mathrm{m},Q}+P),Q;r\,|\,\Xi_1\,|v\rangle\,|^2}{\langle v\,|\,v\rangle} \right. \\
&\qquad\qquad \left. + e^{i(P_{\mathrm{m},Q}-P)x}\, \frac{|\langle (P_{\mathrm{m},Q}-P),Q;r\,|\,\Xi_1\,|v\rangle\,|^2}{\langle v\,|\,v\rangle} \right\} \\
&= e^{iP_{\mathrm{m},Q}x} \sum_r \int\limits_0^{\pi} \mathrm{d}P\, 2\cos(Px)\, \frac{|\langle (P_{\mathrm{m},Q}+P),Q;r\,|\,\Xi_1\,|v\rangle\,|^2}{\langle v\,|\,v\rangle}
\end{aligned} \tag{5.4.12}$$

where the last equality follows from (5.4.11). This shows that $C_\Xi(x)$ is of the form

$$C_\Xi(x) = e^{\frac{2\pi i x}{L}} f(x) \tag{5.4.13}$$

with L satisfying (5.4.9) and $f(x)$ is given by the remaining integral in (5.4.12) which is clearly real. $\square$

Remarks:

1) Note that theorem VI is true for more general Hamiltonians $H(P,Q)$, but it covers in particular the case (5.4.7) for the $\mathbb{Z}_n$-chiral Potts model.
2) Note that if the Hamiltonian has several different $P_{\mathrm{m},Q}$ such that (5.4.8) holds (which applies to (5.4.7)) one obtains different expressions for $C_\Xi(x)$ involving different L and $f(x)$. We have argued before that form factors are maximal for smallest energy. Therefore one may expect to obtain the representation with $f(x) > 0$ on $x \in [0,y]$ with maximal y choosing the value $P_{\mathrm{m},Q}$ that corresponds to the *minimum* of the dispersion relation of the fundamental particle.

From lemma I and theorem VI we immediately obtain the following

Corollary:

$$C_{\Gamma^Q}(x) = e^{\frac{2\pi i x}{L}} f_{Q,r}(x) \tag{5.4.14a}$$

with

$$\begin{aligned} f_{Q,r}(x) &\in \mathbb{R} && \forall x\,, \\ L &= \infty && \text{for } \phi = r\pi, r \in \mathbb{Z} \text{ or } \varphi \in \mathbb{R}, \mathrm{Re}(\phi) = 0\,, \\ L &= \frac{2n}{n-2Q} && \text{for } \varphi \in \mathbb{R}, \mathrm{Re}(\phi) = \pi \text{ and } 0 < Q < n\,. \end{aligned} \tag{5.4.14b}$$

Il libro della natura é scritto in lingua matematica

Galileo Galilei

6. Extended conformal algebras

Symmetries play a fundamental rôle in theoretical physics because they help to simplify a problem considerably or sometimes they even determine the relevant quantities completely. For example, the symmetry group $SO(4)$ of the quantum mechanical central force problem allows to determine the spectrum of the hydrogen atom by purely algebraic computations. In particular, for quantum field theories it is desirable to have a sufficiently large symmetry because they can be solved directly in only very few cases. Such a situation does indeed arise in two space-time dimensions where so-called 'extended conformal algebras' (also called $\mathcal{W}$-algebras) provide infinite symmetries. The study of the representation theory of these algebras gives rise to 'rational conformal field theories' (RCFTs) which are in some sense finite. Particular RCFTs describe the second order phase transitions in $\mathbb{Z}_n$-spin chains as we have already mentioned earlier. More generally, a classification of RCFTs would also classify the associated conformally invariant critical points of statistical models. Therefore, it is interesting to understand the structure of RCFTs. This also involves a good understanding of $\mathcal{W}$-algebras and the RCFTs associated to them (their so-called 'rational models'). The remainder of this thesis is devoted to investigations that either yield new results on the structure of $\mathcal{W}$-algebras or are relevant for spin quantum chains.

6.1. Quantum $\mathcal{W}$-algebras

In this section we give a brief review of the notion of a quantum $\mathcal{W}$-algebra – for details see e.g. [33, 55].

The ingredients of a quantum $\mathcal{W}$-algebra are:

1) A quantum $\mathcal{W}$ algebra is a vector space of local chiral quantum fields, i.e. there is a basis of fields $\phi(z)$ depending on a complex coordinate $z \in \overline{\mathbb{C}}$ (including one point at infinity) with definite '*conformal dimension*' $d(\phi)$ and mode expansion

$$\phi(z) = \sum_{n-d(\phi)\in\mathbb{Z}} z^{n-d(\phi)} \phi_n \tag{6.1.1}$$

such that all fields $\phi(z)$ are either bosonic or fermionic and that their dimensions are half-integer $2d(\phi) \in \mathbb{Z}$.

2) The algebraic structure is encoded in the so-called 'operator product expansion' (OPE) of two fields $\phi(z)$, $\chi(w)$:

$$\phi(z) \circ \chi(w) = \sum_{\psi} \frac{A^{\psi}_{\phi\chi}\psi(w)}{(z-w)^{d(\phi)+d(\chi)-d(\psi)}} \tag{6.1.2}$$

where the sum on the r.h.s. of (6.1.2) runs over all local chiral fields in the $\mathcal{W}$-algebra. The $A^{\psi}_{\phi\chi}$ are the structure constants of the $\mathcal{W}$-algebra. The l.h.s. of (6.1.2) is assumed to be radially ordered. The OPE (6.1.2) is required to be associative. Inserting the mode expansion (6.1.1) into (6.1.2) and performing Cauchy integrals, the singular part of the OPE gives rise to a Lie bracket whereas the regular part defines a normal ordered product $(\phi\partial^n\chi)$ (the derivative ∂ is defined in the obvious manner). Note that the associativity of the OPE can be used in order to compute OPEs involving normal ordered products (also known as 'Wick rules').

3) The $\mathcal{W}$-algebra contains a distinguished field, the energy-momentum tensor L with OPE:

$$L(z) \circ L(w) = \frac{c}{2(z-w)^4} + \frac{2L(w)}{(z-w)^2} + \frac{L'(w)}{(z-w)} + reg. \tag{6.1.3}$$

The constant c is called the '*central charge*'. The Lie algebra obtained by a mode expansion of the singular part of (6.1.3) is a representation of the 'Virasoro algebra' where the central element C is represented by $c\mathbb{1}$.

4) The energy-momentum tensor L defines a grading on the $\mathcal{W}$-algebra:

$$L(z) \circ \phi(w) = \frac{d(\phi)\phi(w)}{(z-w)^2} + \sum_{\substack{\psi \\ d(\psi)\neq d(\phi)}} \frac{A^{\psi}_{L\phi}\psi(w)}{(z-w)^{2+d(\phi)-d(\psi)}} \tag{6.1.4}$$

where $d(\phi)$ is the conformal dimension of ϕ.

5) Fields transforming as

$$L(z) \circ \phi(w) = \frac{d(\phi)\phi(w)}{(z-w)^2} + \frac{\phi'(w)}{(z-w)} + \sum_{\substack{\psi \\ |d(\psi)-d(\phi)|>1}} \frac{A^{\psi}_{L\phi}\psi(w)}{(z-w)^{2+d(\phi)-d(\psi)}} \tag{6.1.5}$$

are called '*quasi-primary*'. The field ϕ is called '*primary*' if the remaining sum runs only over fields ψ with $d(\psi) > d(\phi)+1$. Note that the energy-momentum tensor L itself is quasi-primary with conformal dimension $d(L) = 2$.

6) A basis for all fields in the $\mathcal{W}$-algebra can be obtained from a countable basic set of quasi-primary fields $\{W^{(i)}\}$ using normal ordered products and derivatives. The $W^{(i)}$ are called '*generators*'. If the set of generators is minimal, the $\mathcal{W}$-algebra is called a '$\mathcal{W}(d(W^{(1)}), d(W^{(2)}), \ldots)$'.

7) There is an irreducible representation of the mode algebra, the so-called '*vacuum representation*', i.e. the modes ϕ_n of any field $\phi(z)$ act as endomorphisms in the vacuum representation. The vacuum representation has a cyclic highest weight vector $|v\rangle$ with the property

$$\phi_n\,|v\rangle = 0\,, \qquad \forall n < d(\phi)\,. \tag{6.1.6}$$

A normal ordered differential polynomial that acts trivially in the vacuum representation is identically equal to zero. Fields with this property are called '*null fields*'. Note that it is sufficient to require (6.1.6) for quasi-primary fields only, it then automatically extends to all fields including derivatives.

Property 7) gives a precise meaning to the fields $\phi(z)$. The definition of a $\mathcal{W}$-algebra can be made precise using the mathematical language of vertex operator algebras (see [47] for a definition). Then, property 7) is the starting point of the definition and properties 1) - 6) turn out to be reformulations of the axioms of a vertex operator algebra. In general, one will have to impose additional finiteness conditions like requiring the graded components of the vacuum module to be finite dimensional.

The simplest $\mathcal{W}$-algebras are '*current algebras*'. They are generated by currents $J_i(z)$ (fields with dimension $d(J_i) = 1$) with OPEs

$$J_i(z) \circ J_j(w) = \frac{g_{ij}\, k}{(z-w)^2} + \sum_l \frac{f_{ij}^l\, J_l(w)}{(z-w)} + reg. \tag{6.1.7}$$

where g_{ij} is an invariant metric of some Lie algebra $\mathcal{L}_n$ and the f_{ij}^l are the structure constants of this Lie algebra. The current algebra defined by (6.1.7) is denoted by '$\hat{\mathcal{L}}_n$' and k is called the '*level*'. The singular part of the OPE of the basic currents J_i defines an infinite dimensional Lie algebra which is a so-called 'Kac-Moody algebra'. Below we will abuse notation and also refer to the $\mathcal{W}$-algebras defined by (6.1.7) with the term Kac-Moody algebra. In particular we will ignore that it is not entirely trivial that a Kac-Moody algebra becomes a $\mathcal{W}$-algebra once it is endowed with a normal ordered product.

There are several different constructions for $\mathcal{W}$-algebras, most of them starting from Kac-Moody algebras (6.1.7). The so-called '*coset construction*' (also known as the GKO construction since for $\hat{\mathcal{L}}_n = \widehat{sl(2)}$ it is the construction for representations of the Virasoro algebra (6.1.3) of ref. [78]) is particularly simple to formulate. There are two closely related types of cosets:

$$\frac{W}{\hat{\mathcal{L}}_n}, \qquad\qquad \frac{W}{\mathcal{L}_n}. \tag{6.1.8}$$

By definition, the coset $\mathcal{W}$-algebra $W/\hat{\mathcal{L}}_n$ is formed by all fields in the $\mathcal{W}$-algebra W that commute (i.e. have regular OPEs) with the Kac-Moody subalgebra $\hat{\mathcal{L}}_n \subset W$. Similarly, the coset $W/\mathcal{L}_n$ is defined as the set of all fields in W that are invariant with respect to the action of the Lie algebra $\mathcal{L}_n$ implemented by the zero modes of the currents $\hat{\mathcal{L}}_n \subset W$. If the energy-momentum tensor does not coincide with the Sugawara energy-momentum tensor of $\hat{\mathcal{L}}_n$, the coset (6.1.8) yields automatically a closed $\mathcal{W}$-subalgebra of W (see e.g. [33] for more details).

Another very important construction is the so-called '*quantized Drinfeld-Sokolov*' (DS) reduction (see e.g. [32, 60] for recent descriptions). This reduction is a Hamiltonian reduction that also gives a precise meaning to the 'quantized Miura map' of the Fateev-Luk'yanov construction (see e.g. [54, 55]). Here we just recall some ingredients – for details see e.g. [32, 60]. The data specifying the DS reduction is an embedding of $sl(2)$ into $\mathcal{L}_n$. The Cartan generator H of the $sl(2)$ defines a grading on $\mathcal{L}_n$. By definition, the positive step operator E_+ of this $sl(2)$ has grade one. Let T^j be the basis of $\mathcal{L}_n$ with the metric g_{ij} and structure constants f_{ij}^l used in (6.1.7). We introduce a Lie algebra valued current (J) by $(J) = \sum_j J_j T^j$. The grading on $\mathcal{L}_n$ leads to the following decomposition of the Kac-Moody algebra

$$(J) = (J)_- \oplus (J)_0 \oplus (J)_+ \tag{6.1.9}$$

where $(J)_0$ refers to the currents of grade zero, $(J)_-$ to all currents with *arbitrary* negative grade and $(J)_+$ to the currents with arbitrary positive grade. The DS reduction is defined by imposing the following first class constraints on the currents with positive grade [5]):

$$(J)_+ = E_+ \,. \tag{6.1.10}$$

This amounts to equating the positive grade currents to zero except for the one corresponding to E_+ that is set to one. From a classical point of view the constraints (6.1.10) generate gauge transformations and the problem is to find a suitable representative for each gauge orbit. At the quantum level the constraints (6.1.10) are imposed using a nilpotent BRST operator $Q_{\rm BRST}$ ($Q_{\rm BRST}^2 = 0$). In order to impose the constraints with a BRST operator one has to introduce some auxiliary fields, so-called ghost-antighost pairs. Then one considers the cohomology of $Q_{\rm BRST}$ and the problem is to find a suitable representative for each cohomology class.

Suitable representatives are associated to the so-called lowest weight gauge: The generators $W^{(j)}$ of the DS $\mathcal{W}$-algebra can be chosen to be the lowest weight components of the embedded $sl(2)$ in the adjoint representation on the Kac-Moody algebra $\hat{\mathcal{L}}_n$. From the lowest weight gauge one reads off that the conformal dimension of $W^{(j)}$ is given by the spin S_j of the $sl(2)$ representation, i.e. $d(W^{(j)}) = S_j + 1$. Furthermore, the generators can be made primary using a certain 'dressing'. In the quantum case, this dressing is provided by the 'tic-tac-toe' equations of [32].

For the principal embedding of $sl(2)$ into $\mathcal{L}_n$ the DS reduction gives rise to the so-called Casimir $\mathcal{W}$-algebras which we denote by $\mathcal{WL}_n$. In the case of a nonprincipal $sl(2)$ embedding into a simple Lie algebra $\mathcal{L}_n$ we use the notation $\mathcal{W}_{\mathcal{S}}^{\mathcal{L}_n}$ where $\mathcal{S}$ denotes the embedding. For example, for $\mathcal{L}_n = \mathcal{A}_n$, $\mathcal{S}$ can be chosen as the r-tuple of the dimensions of the irreducible $sl(2)$ representations which appear in the defining representation of $\mathcal{L}_n$. The Polyakov-Bershadsky algebra $\mathcal{W}(1, \frac{3}{2}, \frac{3}{2}, 2)$ [116, 25] which is obtained by DS reduction of the nonprincipal $sl(2)$ embedding into $sl(3)$ is abbreviated in this notation by $\mathcal{W}_{2,1}^{sl(3)}$.

In the next section we shall be interested in non-trivial outer automorphisms of $\mathcal{W}$-algebras and their effect on the HWRs. An automorphism ρ of a $\mathcal{W}$-algebra is a bijective map of the algebra that satisfies the following compatibility condition with (6.1.2):

$$\rho(\phi(z)) \circ \rho(\chi(w)) = \sum_{\psi} \frac{A_{\phi\chi}^{\psi} \rho(\psi(w))}{(z-w)^{d(\phi)+d(\chi)-d(\psi)}} \,. \tag{6.1.11}$$

ρ is called an 'outer' automorphism if it is not generated by the $\mathcal{W}$-algebra itself. Each such automorphism enables one to impose non-trivial boundary conditions on the fields ϕ_j in the algebra:

$$\phi_j\left(e^{2\pi i} z\right) = \rho\left(\phi_j\left(z\right)\right) \tag{6.1.12}$$

where now the argument z lives on a suitable covering of the complex plane. This type of boundary condition will be called a 'twist'.

[5]) There are some subtleties for the grade $\frac{1}{2}$ part of a half-integral embedding which we ignore here because it is not relevant for the aspects we need below.

Quite often automorphisms ρ have the form $\rho(W_j(z)) = \pm W_j(z)$ where some generators $W_j(z)$ transform with a plus sign and others with a minus sign. For any field with $\phi_j\left(e^{2\pi i}z\right) = -\phi_j(z)$ the Laurent expansion (6.1.1) has to be modified to

$$\phi_j(z) = \sum_{n-d(\phi_j)\in\mathbb{Z}+\frac{1}{2}} z^{n-d(\phi_j)}\phi_{j,n}\,. \tag{6.1.13}$$

This leads to the Ramond-sector of a fermionic $\mathcal{W}$-algebra. Bosonic fields acquire half-integer modes.

In the presence of an outer automorphism one can also consider the projection of the $\mathcal{W}$-algebra onto the invariant subspace. This projection is called an '*orbifold*'.

6.2. Automorphisms of Casimir $\mathcal{W}$-algebras and boundary conditions

The simplest $\mathcal{W}$-algebras are those with one additional generator, so-called '$\mathcal{W}(2,\delta)$-algebras'. The automorphisms of these algebras were studied in detail in [90] and [88]. Here we will focus on the so-called 'Casimir' algebras $\mathcal{WL}_n$ where the dimensions of the simple fields equal the orders of the Casimir invariants of a simple Lie algebra $\mathcal{L}_n$ (see e.g. [15, 16]). One common approach to their study is Toda field theory [19, 20, 26]. As we will see below only Casimir algebras $\mathcal{WL}_n$ based on *simply-laced* $\mathcal{L}_n$ have non-trivial outer automorphisms for generic c. The unitary minimal series of these algebras can also be studied via GKO-constructions [78]. Q. Ho-Kim and H.B. Zheng have noticed that in this approach outer automorphisms of the Lie algebra give rise to automorphisms of the $\mathcal{W}$-algebra and argued that there no further ones [85, 86, 87]. Owing to their work twists of the unitary minimal series of Casimir algebras are well understood. Still, we would like to comment on Casimir algebras from the point of view of extended conformal algebras, including the non-unitary minimal models into our discussion.

One way to study automorphisms of Casimir $\mathcal{W}$-algebras is by inspection of the structure constants of known examples. Inspecting the structure constants of the algebras constructed e.g. in [30, 102, 93, 94] it was observed in [90] that $\mathcal{WL}_n$ with generic central charge c has as many automorphisms as $\mathcal{L}_n$ has. This was also observed before for the *unitary minimal series* in [85, 86, 87]. In fact, it can easily be seen that using quantized Drinfeld Sokolov (DS) reduction (see e.g. [32, 60]) each outer automorphism of the underlying Lie algebra gives rise to an automorphism of the associated Casimir $\mathcal{W}$-algebra. In the DS framework Casimir $\mathcal{W}$-algebras arise from the principal $sl(2)$ embedding. The Cartan- resp. step-operators of this principal $sl(2)$ are sums over all the Cartan- resp. step-operators associated to the simple roots of the underlying Lie algebra. Since outer automorphisms of simple Lie algebras are nothing but certain permutations of the roots the principal $sl(2)$ is clearly preserved. Therefore, the automorphism of the underlying Lie (or Kac-Moody) algebra survives the reduction. We will argue below for $\mathcal{WA}_n$ that the automorphism remains non-trivial after the reduction. In the case of Casimir $\mathcal{W}$-algebras it seems that this type of automorphism is in fact the only one [90] although this is far from being obvious. In fact, also $\mathcal{W}$-algebras for *non-principal* $sl(2)$ embedding admit automorphisms some of which do not seem to have any relation to the automorphisms of the underlying Lie algebra (compare e.g. the analogue of the Ramond sector of the Polyakov-Bershadsky-algebra $\mathcal{W}(1, \frac{3}{2}, \frac{3}{2}, 2)$ [116, 25]).

In the case of $\mathcal{WA}_n$ the effect of the automorphism of the underlying Lie algebra after reduction can easily be controlled. To this end one uses the lowest weight gauge for the DS reduction, i.e. one has to find the lowest weights of the principal $sl(2)$ in the adjoint representation. These lowest weights are given by the tensor product of a spin $\frac{n}{2}$ representation with itself minus a spin zero representations (in order to ensure tracelessness). By inspection of the Clebsch-Gordan coefficients one sees that the parity under the automorphism alternates with the spin S, i.e. the lowest weights transform with a factor $(-1)^S$. Since the dimension of the generating fields $W^{(j)}$ is $d(W^{(j)}) = S_j + 1$ and the energy-momentum tensor $L = W^{(1)}$ must be invariant, one sees that the generators with even dimension are invariant and those with odd dimension pick up a minus sign. This shows that

$$\rho(W^{(j)}) = (-1)^{d(W^{(j)})} W^{(j)} \tag{6.2.1}$$

for the generators $W^{(j)}$ of $\mathcal{WA}_n \cong \mathcal{W}(2, \ldots, n+1)$.

For certain values of the central charge one finds null fields in the algebras $\mathcal{WA}_2 \cong \mathcal{W}(2, 3)$ and $\mathcal{WA}_3 \cong \mathcal{W}(2, 3, 4)$. These can be exploited to determine the conformal dimensions of some minimal models along the lines of [48, 123] using the special purpose computer algebra system [89]. Certain normal ordered products in the twisted sector are not straightforward to handle (see e.g. [50] for a discussion of problems of this type) only a few models are accessible to these direct computations. The results have been presented in [90]. Here, we list only the subset of results corresponding to $\mathbb{Z}_n$ parafermions (see table 5).

$\mathcal{W}(2,3)$	$c = \frac{4}{5}$	$\mathcal{W}(2,3,4)$		$c = 1$
untwisted	*twisted*	*untwisted*		*twisted*
0	$\frac{1}{8}$	0	$\frac{3}{4}$	$\frac{1}{16}$
$\frac{2}{3}$	$\frac{1}{40}$	1	$\frac{9}{16}$	$\frac{3}{16}$
$\frac{2}{5}$		$\frac{1}{3}$	$\frac{1}{16}$	$\frac{1}{48}$
$\frac{1}{15}$		$\frac{1}{12}$		$\frac{25}{48}$

Table 5: Conformal dimensions of untwisted and twisted $\mathcal{W}(2,3) \cong \mathcal{WA}_2$ and $\mathcal{W}(2,3,4) \cong \mathcal{WA}_3$ for the $\mathbb{Z}_3$ resp. $\mathbb{Z}_4$ parafermionic models $c_{\mathcal{A}_2}(4,5) = \frac{4}{5}$, $c_{\mathcal{A}_3}(5,6) = 1$.

From the above discussion we conclude that there will be no outer automorphisms for $\mathcal{WA}_1$, $\mathcal{WB}_n$, $\mathcal{WC}_n$, $\mathcal{WE}_7$, $\mathcal{WE}_8$, $\mathcal{WF}_4$ and $\mathcal{WG}_2$. The algebras $\mathcal{WA}_n$ for $n > 1$, $\mathcal{WD}_n$ for $n > 4$ and $\mathcal{WE}_6$ should have exactly one outer automorphism and correspondingly exactly one twisted sector in addition to the untwisted one. For these algebras explicit computations [90] showed how the formulae for the h-values in [86, 87] might generalize:

$$\begin{aligned} c_{\mathcal{L}_n}(p,q) &= n - 12\rho^2 \frac{(p-q)^2}{pq} \, , \\ h^{\mathcal{L}_n^{(1,2,3)}}_{p,q;\lambda,\mu} &= \frac{(p\lambda - q\mu)^2}{2pq} + \frac{c^{\mathcal{L}_n}_{p,q} - n}{24} + \tilde{h} n_1 \, , \end{aligned} \tag{6.2.2}$$

where

$$\rho = \sum_{i=1}^{n} \tilde{\Omega}_i \ , \qquad \lambda = \sum_{i=1}^{n_0} r_i \Omega_i \ , \qquad \mu = \sum_{i=1}^{n_0} s_i \Omega_i \ , \tag{6.2.3}$$

and n_0, n_1 are the dimensions of the invariant subalgebra $\mathcal{L}'_{n_0}$ respectively twisted subalgebra of $\mathcal{L}_n$; $\tilde{\Omega}_i$ are the fundamental weights of $\mathcal{L}_n$; Ω_i the fundamental weights of $\mathcal{L}'_{n_0}$; $\tilde{h}$ is a constant (that can be interpreted as the conformal dimension of some field) and r_i, s_i positive integers subject to certain constraints. For the case of $\mathcal{A}_n$ the invariant subalgebra is $\mathcal{C}_{[\frac{n+1}{2}]}$. In the unitary minimal series of $\mathcal{WA}_n$, $\mathcal{WD}_n$ $(n > 4)$ and $\mathcal{WE}_6$ one has $\tilde{h} = \frac{1}{16}$. We observe that (6.2.2) indeed reproduces the data in table 5 for $\mathcal{W}(2,3,4)$ if we use the weights of $\mathcal{C}_2$ (which is the invariant subalgebra) and $\tilde{h} = \frac{1}{16}$.

For $\mathcal{L}_n^{(1)}$ (periodic boundary conditions) eqs. (6.2.2) with (6.2.3) have been rigorously proven in [63] (see e.g. [28] for a brief summary including the range of the integers r_i and s_i). It should be possible to generalize the result of [63] to twisted Kac-Moody algebras $\hat{\mathcal{L}}_n^{(2)}$ and $\hat{\mathcal{D}}_4^{(3)}$ yielding a rigorous derivation of (6.2.2) with (6.2.3). At least one thing is immediately clear if one assumes that the representations of a (twisted) $\mathcal{W}$-algebra obtained by DS reduction are induced by admissible representations of the (twisted) Kac-Moody algebra: The representations of a Kac-Moody algebra are labeled by the weights of the Lie algebra formed by the zero modes of all currents. While for an untwisted Kac-Moody algebra $\hat{\mathcal{L}}_n^{(1)}$ the algebra of zero modes is isomorphic to $\mathcal{L}_n$, the zero modes of a *twisted* Kac-Moody algebra form a Lie algebra $\mathcal{L}'_{n_0}$ that is precisely the *invariant* subalgebra of $\mathcal{L}_n$.

The exceptional cases $\mathcal{WE}_6$ and $\mathcal{WD}_4$ are particularly interesting. Especially for $\mathcal{WD}_4 \cong \mathcal{W}(2,4,4,6)$ the group of outer automorphisms should be $\mathcal{S}_3$ for generic c. In $\mathcal{W}(2,4,4,6)$ one structure constant remains a free parameter [101]. It was observed in [90] that one can define an operation of $O(2)$ on the two generators of conformal dimension 4 under which the structure constants transform covariant. The algebra is *invariant* under the natural embedding of $\mathcal{S}_3$ into the group $O(2)$ operating on the fields if one chooses the self coupling constants of these two generators to be equal.

Denote the primary fields of dimension 4 in $\mathcal{W}(2,4,4,6)$ by $V(z)$ and $W(z)$. Then the $\mathcal{S}_3$-symmetry of this algebra translates into the following type of boundary conditions for the given choice of coupling constants:

$$\begin{aligned} V(e^{2\pi i}z) &= \cos(\alpha)V(z) - \sin(\alpha)W(z) \\ W(e^{2\pi i}z) &= \sin(\alpha)V(z) + \cos(\alpha)W(z) \end{aligned} \tag{6.2.4}$$

or

$$\begin{aligned} V(e^{2\pi i}z) &= \cos(\alpha)W(z) - \sin(\alpha)V(z) \\ W(e^{2\pi i}z) &= \sin(\alpha)W(z) + \cos(\alpha)V(z) \end{aligned} \tag{6.2.5}$$

with $\alpha \in \{0, \frac{2}{3}\pi, \frac{4}{3}\pi\}$. The three different boundary conditions given by (6.2.4) correspond to those elements of $\mathcal{S}_3$ which under the embedding yield elements of $SO(2)$. The boundary conditions (6.2.5) correspond to the three elements of $\mathcal{S}_3$ that are mapped to elements in $O(2)$ with determinant -1.

The h-values in the unitary minimal series (6.2.2) of $\mathcal{WD}_4$ have been calculated in [86] without having to consider the boundary conditions of the additional simple fields which look quite strange at first sight. Note that for $\mathcal{D}_4$ the invariant subalgebra is the exceptional algebra $\mathcal{G}_2$ and here $\tilde{h}$ in (6.2.2) satisfies $\tilde{h} = \frac{1}{18}$.

In [33] it has already been stated that the $\mathcal{S}_3$-symmetry should lead to modes in $\frac{\mathbb{Z}}{3}$ and the precise statement was presented in [90] which we now would like to recall. Let us first focus on (6.2.4). Set $U^{(1)}(z) := V(z) + iW(z)$ and $U^{(2)}(z) := V(z) - iW(z)$. Then (6.2.4) turns into $U^{(1)}(e^{2\pi i}z) = e^{i\alpha}U^{(1)}(z)$ and $U^{(2)}(e^{2\pi i}z) = e^{-i\alpha}U^{(2)}(z)$ which can be satisfied by choosing modes in $\mathbb{Z} + \frac{\alpha}{2\pi}$ for $U^{(1)}$ and those for $U^{(2)}$ in $\mathbb{Z} - \frac{\alpha}{2\pi}$. Consider now (6.2.5). For this case set $Y^{(1)}(z) := \cos(\alpha)V(z) + (\sin(\alpha)+1)W(z)$ and $Y^{(2)}(z) := \cos(\alpha)V(z) + (\sin(\alpha) - 1)W(z)$. Now (6.2.5) turns into $Y^{(1)}(e^{2\pi i}z) = Y^{(1)}(z)$ and $Y^{(2)}(e^{2\pi i}z) = -Y^{(2)}(z)$. This can be satisfied by choosing the modes for $Y^{(1)}$ in $\mathbb{Z}$ and those for $Y^{(2)}$ in $\mathbb{Z} + \frac{1}{2}$.

We would like to conclude this discussion by commenting on the relation of twisted representations to orbifolds (for a detailed discussion of orbifolding see e.g. [44]). For $\mathcal{W}$-algebras with a $\mathbb{Z}_2$ automorphism $\rho^2 = \mathbb{1}$ one has two partition functions, one where only the characters $\chi^W = \mathrm{tr}_V q^{L_0 - \frac{c}{24}}$ of the untwisted sector enter, and one where the characters χ^W *and* $\tilde{\chi}^W = \mathrm{tr}_V \rho q^{L_0 - \frac{c}{24}}$ of both sectors enter. The latter can be identified with the partition function Z of the orbifold [6]):

$$
\begin{aligned}
Z &= \sum_{k:\ \mathrm{untwisted}} \left[(\chi_k^W)^* \chi_k^W + (\tilde{\chi}_k^W)^* \tilde{\chi}_k^W\right] + \sum_{k:\ \mathrm{twisted}} \left[(\chi_k^W)^* \chi_k^W + (\tilde{\chi}_k^W)^* \tilde{\chi}_k^W\right] \\
&= 2 \sum_{\substack{k:\ \mathrm{untwisted} \\ \mathrm{and\ twisted}}} \left[\tfrac{1}{2}(\chi_k^W + \tilde{\chi}_k^W)^* \tfrac{1}{2}(\chi_k^W + \tilde{\chi}_k^W) + \tfrac{1}{2}(\chi_k^W - \tilde{\chi}_k^W)^* \tfrac{1}{2}(\chi_k^W - \tilde{\chi}_k^W)\right] .
\end{aligned} \tag{6.2.6}
$$

This implies that the characters of the orbifold $\mathcal{W}$-algebra are given by $\frac{1}{2}(\chi_k^W + \tilde{\chi}_k^W)$ and $\frac{1}{2}(\chi_k^W - \tilde{\chi}_k^W)$. We conclude that the h-values for the HWRs of the orbifold are those of the original $\mathcal{W}$-algebra in both sectors in addition to some which differ by (half-) integers.

It would be interesting to generalize the observations of this section to the supersymmetric case. Of special interest is $osp(4|4)$ which is the supersymmetric analogon of $\mathcal{D}_4$. The corresponding Casimir algebra is a $\mathcal{SW}(\frac{3}{2}, 2, 2, \frac{7}{2})$. In [90] it was argued on the basis of some explicit results in [29] that $\mathcal{SW}(\frac{3}{2}, 2, 2, \frac{7}{2})$ should be invariant under the natural embedding of $\mathcal{S}_3$ into the group $O(2)$ operating on the fields if one chooses the self coupling constants of the two generators of dimension two to be equal – precisely like for $\mathcal{WD}_4 \cong \mathcal{W}(2, 4, 4, 6)$.

6.3. Consequences for spin quantum chains

As already pointed out in [85] there is a close connection of the partition function of $\mathcal{W}(2, 3)$ at $c = \frac{4}{5}$ including the twisted sector and the three states Potts model. In fact, the different boundary conditions of $\mathcal{W}(2, 3)$ correspond to the different boundary conditions of the Potts quantum spin chain at critical temperature. Choosing the spin shift operator at the end of the chain to be equal to the spin shift operator at the first site yields the

[6]) We simplify notation by absorbing multiplicities of characters into the index set.

field content of the 'untwisted' sector of $\mathcal{W}(2,3)$ (see e.g. [57, 133] and [71] for numerical verification). We recall the remarkable fact [85] that the twisted sector of $\mathcal{W}(2,3)$ yields additional representations which can be identified with fields in the thermodynamic limit of the three states Potts quantum spin chain if the spin shift operator at the end of the chain is chosen to equal the adjoint of the one at the first site [37].

It would be interesting to know if this observation generalizes to *all* $\mathbb{Z}_n$. For twisted boundary conditions only partial results are available in the literature (see e.g. [74]). We shall therefore present an explicit verification of this statement in the case of $\mathbb{Z}_4$. We will follow the approach of [71] and study the spectrum Hamiltonian (3.1.1) at $\phi = \varphi = 0$ numerically.

Let $E_{N,i}$ be the eigenvalues of $H_N^{(n)}$ with periodic boundary conditions in ascending order and $\tilde{E}_{N,i}$ those with twisted boundary conditions. Then the relevant scaling functions are given by [36, 72]:

$$\begin{aligned} \xi_{N,i} &:= \frac{N}{2\pi}(\tilde{E}_{N,i} - E_{N,0}) \\ \xi_i &:= \lim_{N\to\infty} \xi_{N,i}. \end{aligned} \tag{6.3.1}$$

In the case of periodic and cyclic boundary conditions, the eigenvalues Q of the charge operator (3.1.9) and momentum P are good quantum numbers. In the case of twisted boundary conditions neither charge nor momentum are conserved any more and one does not have any obvious conserved quantities. At least for even n the charge Q mod 2 is conserved.

Assume that (3.1.1) with $\phi = \varphi = 0$ exhibits conformal invariance at $\lambda = 1$ and denote the dimensions of the fields in the left chiral part by h and of those in the right chiral part by $\bar{h}$. For periodic and twisted boundary conditions the field theory is diagonal, i.e. the fields $\phi(z,\bar{z})$ with dimension $h+\bar{h}$ satisfy $h = \bar{h}$ and thus have vanishing spin $h - \bar{h}$. Therefore, the modes of the fields $\phi(z,\bar{z})$ yield levels in the spectrum with $\xi = h + \bar{h} + r$ where $r \in \mathbb{Z}_+$ for periodic boundary conditions and $r \in \frac{\mathbb{Z}_+}{2}$ for twisted boundary conditions.

In order to test this method we shall first study the well-known three states Potts model. For $\mathbb{Z}_3$ we have studied 3 to 9 sites. Thus, it was necessary to partially diagonalize matrices of dimension $3^9 = 19683$. The limits $N \to \infty$ of the lowest gaps ξ_i are given in table 6.

$\mathbb{Z}_3$		
i	ξ_i	$h + \bar{h} + r$
0	0.050000(2)	$\frac{1}{40} + \frac{1}{40}$
1	0.250005(5)	$\frac{1}{8} + \frac{1}{8}$
2	0.5500(5)	$\frac{1}{40} + \frac{1}{40} + \frac{1}{2}$
3	1.05(4)	$\frac{1}{40} + \frac{1}{40} + 1$

Table 6: The low-lying spectrum of the twisted $\mathbb{Z}_3$-chain at $\lambda = 1$

The numbers in brackets indicate the estimated error in the last given digit. For details on the extrapolation procedures and error estimation see e.g. [84]. We do not give more than four levels because the errors of the next levels make an accurate identification impossible. Note that we can nicely identify the dimensions $\frac{1}{40}$ and $\frac{1}{8}$ of the chiral fields – as expected.

Let us now turn to $\mathbb{Z}_4$. The spectrum of the $\mathbb{Z}_4$-chain was already discussed in [14] also for twisted boundary condition. This was done applying Kac-Moody algebra and numerical techniques. Since the former considerations are analogous to the discussion of the previous section and the numerical results are unpublished, we will present results of a direct calculation here because we would like to demonstrate the correspondence between boundary conditions in statistical mechanics and conformal field theory. Note that the $\mathbb{Z}_4$-version of (3.1.1) at $\phi = \varphi = 0$ is a special case of the Ashkin-Teller quantum chain which was introduced in [98] setting the parameter $h = \frac{1}{3}$ (in the notations of [13]).

For $\mathbb{Z}_4$ we have at least a splitting of the spectrum into two sectors of Q mod 2. We have studied 4 to 8 sites, implying the partial diagonalization of matrices in dimensions up to $4^8/2 = 32768$.

$\mathbb{Z}_4$					
Q mod $2 = 0$			Q mod $2 = 1$		
i	ξ_i	$h+\bar{h}+r$	i	ξ_i	$h+\bar{h}+r$
0	0.04167(2)	$\frac{1}{48}+\frac{1}{48}$	0	0.1254(1)	$\frac{1}{16}+\frac{1}{16}$
1	0.375(2)	$\frac{3}{16}+\frac{3}{16}$	1	0.6231(3)	$\frac{1}{16}+\frac{1}{16}+\frac{1}{2}$
2	1.040(2)	$\frac{25}{48}+\frac{25}{48}$	2	0.623(7)	$\frac{1}{16}+\frac{1}{16}+\frac{1}{2}$
			3	1.12(1)	$\frac{1}{16}+\frac{1}{16}+1$

Table 7: The low-lying spectrum of the twisted $\mathbb{Z}_4$-chain at $\lambda = 1$

The dimensions $\frac{1}{48}$, $\frac{1}{16}$, $\frac{3}{16}$ and $\frac{25}{48}$ of the chiral field theory can be nicely seen in the explicit results of table 7.

The field content of the $\mathbb{Z}_n$-spin quantum chains (3.1.1) at their second order phase transition $\phi = \varphi = 0$, $\lambda = 1$ is given by the first unitary representation of $\mathcal{WA}_{n-1}$, i.e. by (6.2.2) with $\hat{\mathcal{L}}_{n_0-1} = \mathcal{L}_{n-1} = \mathcal{A}_{n-1}$ and $p = n+1$, $q = n+2$. In particular, the central charge for a $\mathbb{Z}_n$-model equals $c = \frac{2(n-1)}{n+2}$. In this section we have explicitly verified for $n = 3$ and 4 that the representations of the twisted sector of $\mathcal{WA}_{n-1}$ correspond to the spectrum of the $\mathbb{Z}_n$-model with twisted boundary conditions. In fact, this is also true for the $\mathbb{Z}_5$-version [65]. These explicit results are in agreement with the statement that the field content of the spin quantum chain (3.1.1) at $\phi = \varphi = 0$, $\lambda = 1$ with twisted boundary conditions $\Gamma_{N+1} = \Gamma_1^+$ can be described by a representation of a twisted $\mathcal{WA}_{n-1}$ for all n. Thus, it is possible to calculate the spectrum of the twisted $\mathbb{Z}_n$-quantum chain by (6.2.2) using $\mathcal{L}_{n-1} = \mathcal{A}_{n-1}$, $\hat{\mathcal{L}}_{n_0} = \mathcal{C}_{[\frac{n}{2}]}$ and $p = n+1$, $q = n+2$.

For cyclic boundary conditions ($\Gamma_{N+1} = \omega^{-R}\Gamma_1$, $0 < R < n$) the diagonal symmetry of the statistical mechanics model is known to be broken such that the spin $h - \bar{h}$ takes on rational values. The dimensions of the chiral fields, however, are unaffected by this change of boundary conditions. This has been verified in [37] and [71] for the case $n = 3$, in [14] for

$n = 4$ and more abstractly for general n in [77]. In [37] a similar result has been obtained for $\Gamma_{N+1} = \omega^{-R}\Gamma_1^+$, $0 < R < 3$, $n = 3$ and the only effect of a factor ω^{-R} for all n should be to combine the left- and right-chiral parts in a non-diagonal way.

We would like to conclude by mentioning that the case of *free* boundary conditions should be described by the representations of the orbifold of $\mathcal{WA}_{n-1}$ at its first unitary minimal model. This can be read off from the one-to-one correspondence of boundary conditions of $\mathcal{W}$-algebras and spin chains which we have just observed. After mapping the cylinder on which the CFT lives to a strip in the plane with open ends, only those fields can survive which are *invariant* with respect to transformations at the boundary which implies that precisely the orbifold is expected to survive in the case of free boundary conditions.

6.4. Classical $\mathcal{W}$-algebras and Virasoro structure

In this section we first give a brief review of the notion of classical $\mathcal{W}$-algebras – for details see e.g. [59, 60]. Afterwards, we make some general statements following from Virasoro covariance which are only partially known in the literature.

For a characterizations of a classical $\mathcal{W}$-algebra we closely follow the quantum case – compare section 6.1:

1') A classical $\mathcal{W}$ algebra is a vector space of local chiral classical fields, i.e. there is a basis of fields $\phi(z)$ depending on a complex coordinate $z \in \overline{\mathbb{C}}$ with definite '*conformal dimension*' $d(\phi)$ and mode expansion

$$\phi(z) = \sum_{n-d(\phi)\in\mathbb{Z}} z^{n-d(\phi)}\phi_n \tag{6.4.1}$$

such that all fields $\phi(z)$ are either bosonic or fermionic and that their dimensions are half-integer $2d(\phi) \in \mathbb{Z}$.

2') These fields form a Poisson bracket algebra which we write in OPE form. The '*classical OPE*' of two fields $\phi(z)$, $\chi(w)$ is of the form:

$$\{\phi(z), \chi(w)\} = \sum_{\substack{\psi \\ d(\phi)+d(\chi)>d(\psi)}} \frac{A^{\psi}_{\phi\chi}\psi(w)}{(z-w)^{d(\phi)+d(\chi)-d(\psi)}} + reg. \tag{6.4.2}$$

The $A^{\psi}_{\phi\chi}$ are the structure constants of the classical $\mathcal{W}$-algebra. Instead of the Wick rules of the the quantum case, the classical OPE has the derivation property of Poisson brackets. For example, $\{\phi(z), \chi(w)\psi(w)\} = \chi(w)\{\phi(z), \psi(w)\} + \{\phi(z), \chi(w)\}\psi(w)$. Inserting the mode expansion (6.4.1) into (6.4.2) and performing Cauchy integrals, the classical OPE gives rise to a Lie bracket – like on the quantum level.

3') The classical $\mathcal{W}$-algebra contains a distinguished field, the energy-momentum tensor L with classical OPE:

$$\{L(z), L(w)\} = \frac{c}{2(z-w)^4} + \frac{2L(w)}{(z-w)^2} + \frac{L'(w)}{(z-w)} + reg. \tag{6.4.3}$$

4') The energy-momentum tensor L defines a grading on the classical $\mathcal{W}$-algebra:

$$\{L(z), \phi(w)\} = \frac{d(\phi)\phi(w)}{(z-w)^2} + \sum_{\substack{\psi \\ d(\psi) \neq d(\phi) \\ 2+d(\phi) > d(\psi)}} \frac{A^{\psi}_{L\phi}\psi(w)}{(z-w)^{2+d(\phi)-d(\psi)}} + reg. \tag{6.4.4}$$

where $d(\phi)$ is the conformal dimension of the classical field ϕ.

5') Classical fields transforming as

$$\{L(z), \phi(w)\} = \frac{d(\phi)\phi(w)}{(z-w)^2} + \frac{\phi'(w)}{(z-w)} + \sum_{\substack{\psi \\ d(\phi) > d(\psi)+1}} \frac{A^{\psi}_{L\phi}\psi(w)}{(z-w)^{2+d(\phi)-d(\psi)}} + reg. \tag{6.4.5}$$

are called '*quasi-primary*'. The field ϕ is called '*primary*' if the remaining sum is absent.

6') All classical fields in the classical $\mathcal{W}$-algebra are differential polynomials (with finite order) in a countable basic set of quasi-primary fields $\{W^{(i)}\}$ – the so-called '*generators*' $W^{(i)}$. In general, this differential polynomial ring will not be freely generated but may have relations, i.e. differential polynomials that vanish identically. Note that in contrast to the normal ordered product of the quantum level, the product of two classical fields is (anti-)commutative.

7') The '*phase space*' of the classical $\mathcal{W}$-algebra is the vector space of meromorphic functions from the Riemannian sphere $\overline{\mathbb{C}}$ into the complex numbers $\mathbb{C}$. The classical fields are defined as integral kernels of functionals on this phase space. In particular, all classical OPEs (6.4.2) have to be understood after Cauchy integration with some meromorphic test function.

Note that usually a notation different from the above is used in the literature. Usually one uses the compact manifold S^1 instead of the Riemannian sphere $\overline{\mathbb{C}}$. Then the poles in the OPE are replaced by δ-functions on the r.h.s. of the Poisson brackets. Test functions are smooth square-integrable functions on S^1, not meromorphic functions. However, this is only a minor difference in the point of view since after all we are interested in the algebraic structure of a classical $\mathcal{W}$-algebra, and here both formulations lead to the same results.

The description in section 6.1 of Kac-Moody algebras, cosets, orbifolds and DS reduction apply at the classical level as well with some obvious minor modifications. Therefore we do not explicitly repeat the corresponding discussion of section 6.1.

In contrast to the quantum case one does not have a bilinear form on a classical $\mathcal{W}$-algebra which one can use to prove basic theorem e.g. about the $su(1,1)$ structure of the space of fields. Nevertheless, explicit constructions are known on the quantum level (see e.g. [30]) which can be transferred to classical $\mathcal{W}$-algebras. Then one can use these explicit constructions in order to prove e.g. that the generators of a classical $\mathcal{W}$-algebra can be chosen primary in quite general situations. In the remainder of this section we wish to indicate how this should be done.

A first result is a formula for a quasi-primary projection of two classical fields including some derivatives:

Lemma II: *(Classical quasi-primary product) For any two quasi-primary fields ϕ, χ let*

$$\mathcal{Q}^{(r)}(\phi,\chi) := \sum_{n+m=r} (-1)^n \binom{2d(\phi)+r-1}{m} \binom{2d(\chi)+r-1}{n} (\partial^n \phi)(\partial^m \chi) . \qquad (6.4.6)$$

Then $\mathcal{Q}^{(r)}(\phi,\chi)$ is a quasi-primary field of conformal dimension $d(\phi)+d(\chi)+r$. ∎

In order to prove this statement one has to apply (6.4.4) to the r.h.s. of (6.4.6) and check that it has the correct transformation properties. Of course, an equivalent expression can be obtained by applying a suitable classical limit [28] to the formula for the quantum case [30]. Covariance problems of this type have been treated in the mathematical literature already many years ago. For example, finding the projection of the rth derivative of the product of two modular forms onto a modular form (see e.g. [128]) is equivalent to determining the quasi-primary projection. In fact, we have taken Eq. (6.4.6) from the formula (1) of [128] which is called the 'rth Rankin-Cohen bracket'.

Note that it is possible that the classical quasi-primary product (6.4.6) vanishes identically.

Now we turn to the question of Virasoro covariance of the space of fields of a classical $\mathcal{W}$-algebra. To this end we need a weak property of the generating set. Then we can show by construction that for any $\mathcal{W}$-algebra with this property the space of fields decomposes into quasi-primary fields and derivatives thereof. We will also say that a $\mathcal{W}$-algebra has a quasi-primary basis if it admits such a decomposition.

Def. VII: A classical $\mathcal{W}$-algebra is called 'regularly generated' if for each fixed dimension Δ there are only finitely many generators with conformal dimension less than Δ.

Claim I: *Any classical $\mathcal{W}$-algebra that is regularly generated admits a basis of quasi-primary fields and derivatives thereof.* ∎

This statement should be proven for homogeneous polynomials of a fixed degree in the generators. For the linear polynomials the claim is true by definition. Also for the second order polynomials it is immediately clear that the formula (6.4.6) yields precisely as many linearly independent quasi-primary fields as are needed in order to complement the derivatives to a basis. More precisely, all linear relations among the second order quasi-primary fields are given by $\mathcal{Q}^{(r)}(\phi,\chi) = \pm\mathcal{Q}^{(r)}(\chi,\phi)$ and $\mathcal{Q}^{(r)}(\phi,\phi) = 0$ for ϕ bosonic and r odd or ϕ fermionic and r even. For polynomials of higher degree we forget at the moment about the relations possibly present in the space of fields (they can be imposed at the very end). Then one has to gain control about the action of the derivative. This can e.g. be done by using partitions into different colours (compare [62] for a presentation in the quantum case). Now a basis of the quasi-primary fields can be labeled by these partitions. It remains to be checked that those quasi-primary polynomials associated to the partitions are indeed linearly independent. We leave this inspection for future investigations.

Note that this claim should in particular be valid for $\mathcal{W}$-algebras that are generated by finitely many fields whose dimensions are strictly positive. However, the above argument should apply to regularly generated classical $\mathcal{W}$-algebras without additional effort. Claim

I might be true in even more general situations but this will certainly give rise to extra complications in the proof.

If a classical $\mathcal{W}$-algebra admits a basis of quasi-primary fields and derivatives thereof one can derive a specialization of the classical OPE (6.4.2) when applied to quasi-primary fields:

Lemma III: *([61]) For any classical $\mathcal{W}$-algebra with a quasi-primary basis the Poisson brackets of two classical quasi-primary fields $\phi(z)$, $\chi(w)$ have the form*

$$\begin{aligned}\{\phi(z),\chi(w)\} =& \frac{d_{\phi,\chi}\delta_{d(\phi),d(\chi)}}{(z-w)^{d(\phi)+d(\chi)}} + \sum_{\substack{\psi \text{ quasi-primary} \\ d(\phi)+d(\chi)>d(\psi)}} C_{\phi\chi}^{\psi} \sum_{r=0}^{d(\phi)+d(\chi)-d(\psi)-1} \\ & \frac{\binom{d(\phi)-d(\chi)+d(\psi)+r-1}{r}\partial^r\psi(w)}{r!\binom{2d(\psi)+r-1}{r}(z-w)^{d(\phi)+d(\chi)-d(\psi)-r}} + reg.\end{aligned} \tag{6.4.7}$$

■

This statement is also true at the quantum level (see e.g. [30]), and in fact was first discovered there. It can be proven along different lines. One can either use the realization of L_{-1} as the differential operator $L_{-1}\phi(z) = z(z\partial + 2d(\phi))\phi(z)$ acting on quasi-primary fields $\phi(z)$. Then one uses covariance of (6.4.2) with respect to this differential operator [61]. Equivalently, lemma III can be derived from the Jacobi identity for the Poisson brackets $\{L(y),\{\phi(z),\chi(w)\}\}$ + cyclic = 0 using (6.4.5).

In view of lemma III we can introduce the following shorthand notation for the Poisson brackets of two classical quasi-primary fields ϕ, χ writing only the quasi-primary fields on the r.h.s.:

$$\phi \star \chi = \sum_{\substack{\psi \text{ quasi-primary} \\ d(\phi)+d(\chi)>d(\psi)}} C_{\phi\chi}^{\psi}\psi\,. \tag{6.4.8}$$

The notation (6.4.8) has to be understood in the sense that the arguments and poles have to be re-instituted in the form of (6.4.7). Similarly, the coupling constants involving derivatives can be recovered from (6.4.7) since they are uniquely given by those involving only quasi-primary fields. In this shorthand notation the classical Virasoro algebra (6.4.3) becomes $L \star L = \frac{c}{2} + 2L$.

This shorthand notation is useful for arguing that one can choose the generators of a classical $\mathcal{W}$-algebra primary in a quite general situation.

Claim II: *All generators of a classical $\mathcal{W}$-algebra except for the Virasoro field L can be chosen to be primary if the $\mathcal{W}$-algebra is regularly generated, the Virasoro centre is non-zero $c \neq 0$ and the conformal dimensions of the generators are strictly positive.* ■

A sketch of the proof of this statement is the following: If claim I is true there is a quasi-primary basis according to the assumptions and we can use the shorthand notation (6.4.8). First we note that the generators $W^{(j)}$ of conformal dimension $d(W^{(j)}) < 2$ must already be primary because of the assumptions. Now consider any generator $W^{(j)}$ of conformal dimension $d(W^{(j)}) = 2$. Since $W^{(j)}$ is quasi-primary, the OPE with L must read $L \star W^{(j)} = \alpha_j c + 2W^{(j)}$. Then $\hat{W}^{(j)} = W^{(j)} - 2\alpha_j L$ is primary. For all other dimensions we first observe that

$$\begin{aligned} L \star \mathcal{Q}^{(r)}(L,\phi) = & \binom{d(\phi)+r-1}{r} \frac{c(r+4)!}{12}\phi + (d(\phi)+r+2)\mathcal{Q}^{(r)}(L,\phi) \\ & + \sum_{\substack{\psi,s \\ d(\psi)+s+2 \leq d(\phi)+r}} \alpha^s_{\phi,\psi}\mathcal{Q}^{(s)}(L,\psi) \end{aligned} \tag{6.4.9}$$

The $\alpha^s_{\phi,\psi}$ are certain structure constants. For the generators $W^{(j)}$ of conformal dimension not equal to two, the OPE with L must have the form

$$L \star W^{(j)} = d(W^{(j)})W^{(j)} + \sum_{k \leq d(W^{(j)})-2} \alpha_k \phi^{(k)} \tag{6.4.10}$$

with one quasi-primary field $\phi^{(k)}$ per conformal dimension k. Now we can use (6.4.9) to add fields $\mathcal{Q}^{(r)}(L,\phi^{(k)})$ with suitable parameters. Since there may be further fields ψ of the same dimensions on the r.h.s. of (6.4.9) this procedure may have to be iterated adding further fields with suitable parameters. According to the assumptions there are only finitely many fields below a fixed conformal dimension. Therefore, after adding finitely many counterterms one is left with a linear system of equations that must be solved. Once this system is solved, the generator becomes primary and claim II is verified. From (6.4.9) one obviously needs $c \neq 0$ in order to have an invertible system. For low conformal dimensions (e.g. $d(W^{(j)}) < 4$) one can argue that this system is indeed invertible. The general case may become quite complicated and we will therefore leave the proof of invertibility to future investigations.

We would like to conclude this section by remarking that from here on it is in principle straightforward to construct classical $\mathcal{W}$-algebras by making some assumptions e.g. on the conformal dimensions and then checking Jacobi identities. For example, one can check that there is a unique classical $\mathcal{W}(2,3)$ (up to isomorphism) if the central terms are chosen to be non-zero.

6.5. Classical cosets and orbifolds

In this section we discuss orbifolds and cosets of classical $\mathcal{W}$-algebras. During the attempts to understand a mysterious algebra of type $\mathcal{W}(2,4,6)$ [51] using some classical limit evidence emerged that a classical analogon would need more generators than this quantum $\mathcal{W}$-algebra and that the same statement should be true for the orbifold of of the $N = 1$ quantum super Virasoro algebra (for more details see [28]). It was then argued in [31] that generic classical cosets and orbifolds are –in contrast to the quantum level– infinitely generated and satisfy infinitely many constraints. Let us now briefly summarize the results of [31].

Classical orbifolds are defined in the same manner as they are defined at the quantum level (see the end of section 6.1). Below we restrict to $\mathbb{Z}_2$ automorphisms ρ that act on the finitely many generators $\{W_a \mid a \in \mathcal{I} \cup \mathcal{K}\}$ as follows:

$$\begin{aligned} \rho(W_a) =& W_a \qquad \forall a \in \mathcal{K}\ , \\ \rho(W_b) =& -W_b \qquad \forall b \in \mathcal{I}\ . \end{aligned} \tag{6.5.1}$$

We can divide the index set $\mathcal{I}$ into two subsets: A set $\mathcal{I}_1$ referring to *bosonic* fields and a set $\mathcal{I}_2$ referring to *fermionic* fields transforming nontrivially under the automorphism ρ. It is easy to determine a generating set *classically.* Note that the nontrivial ρ-invariant differential polynomials are even order in the $\{W_b \mid b \in \mathcal{I}\}$. Plainly, every even order polynomial can be regarded as a polynomial in quadratic expressions. Therefore the quadratic expressions formed out of the $\{W_b \mid b \in \mathcal{I}\}$ generate the orbifold together with the invariant fields $\{W_a \mid a \in \mathcal{K}\}$. A redundant set of quadratic generators is given by:

$$X^{i,j}_{b,c} := W^{(i)}_b W^{(j)}_c \qquad b, c \in \mathcal{I},\ 0 \le i, j \in \mathbb{Z} \tag{6.5.2}$$

where $W^{(i)}_b := \partial^i W_b$. The derivative acts on the generators (6.5.2) as follows:

$$\partial X^{i,j}_{b,c} = X^{i+1,j}_{b,c} + X^{i,j+1}_{b,c}. \tag{6.5.3}$$

Using the action of the derivative (6.5.3) and paying attention to the Pauli principle for the fermionic generators, i.e. that fermions have odd Grassmann parity, one can choose the following minimal set of generators for the orbifold:

$$\begin{aligned} & W_a,\ a \in \mathcal{K} && \text{(invariant generators)}, \\ & X^{0,j}_{b,c} := W_b \partial^j W_c, \quad b < c,\ b, c \in \mathcal{I},\ 0 \le j \in \mathbb{Z}, && \\ & X^{0,j}_{d,d} := W_d \partial^j W_d, \quad d \in \mathcal{I}_1,\ 0 \le j \in 2\mathbb{Z} && \text{(square of bosons)}, \\ & X^{0,j}_{e,e} := W_e \partial^j W_e, \quad e \in \mathcal{I}_2,\ 0 < j \in 2\mathbb{Z}+1 && \text{(square of fermions)} \end{aligned} \tag{6.5.4}$$

where '$b < c$' denotes some ordering of the original generators. Eq. (6.5.4) shows that $\mathbb{Z}_2$ orbifolds are always *infinitely* generated at the classical level (if there is one field transforming non-trivially under ρ).

In order to find the complete set of relations we first regard all $W^{(i)}_a$ as independent. The complete set of relations satisfied by the redundant set of generators (6.5.2) is generated by

$$X^{i,j}_{b,c} - \epsilon_{b,c} X^{j,i}_{c,b} = 0, \tag{6.5.5a}$$

$$X^{i,j}_{b,c} X^{k,l}_{d,e} - \epsilon_{c,d} X^{i,k}_{b,d} X^{j,l}_{c,e} = 0, \tag{6.5.5b}$$

where $\epsilon_{b,c} = -1$ if *both* W_b and W_c are fermions, and $\epsilon_{b,c} = 1$ otherwise. (Clearly, choosing certain indices in (6.5.5) equal leads to trivial relations). The proof that (6.5.5) indeed generate all relations is a simple sorting argument. Plainly, a basis for invariant polynomials is given by those differential monomials that have even degree in the generators transforming non-trivially under ρ if the generators are arranged in a suitable order. Obviously, any given monomial in the fields (6.5.2) can be re-sorted into this order using the relations (6.5.5) and (anti-)commutativity of any two fields.

It is straightforward to derive the relations satisfied by the nonredundant set of generators (6.5.4) from (6.5.5). One simply has to recursively apply (6.5.3) (which encodes the action of the derivative) in order to express the relations (6.5.5) in terms of the generators (6.5.4).

Next, we further elaborate some of these relations for two examples. One of the simplest examples of orbifolds is the bosonic projection of the $N = 1$ super Virasoro algebra. The $N = 1$ super Virasoro algebra is the extension of the Virasoro algebra L by a primary dimension $\frac{3}{2}$ fermion G. According to (6.5.4) a nonredundant set of generators for the classical orbifold is

$$L, \qquad \Phi^n := G\partial^n G \qquad \text{for all odd } n. \tag{6.5.6}$$

In particular, this orbifold has one generator at each positive *even* scale dimension. Using the notation of (6.5.4) we have the identification $\Phi^n = X^{0,n}$ if we omit the irrelevant lower indices. From (6.5.5b) one reads off $0 = X^{0,j}X^{0,l} + X^{0,0}X^{j,l} = X^{0,j}X^{0,l}$ because $X^{0,0} = 0$. In terms of the generators (6.5.6) these infinitely many relations read

$$\Phi^n\Phi^m = 0 \qquad \text{for any} \quad 0 < n, m \in 2\mathbb{Z} + 1. \tag{6.5.7}$$

In this case the particular subset (6.5.7) of relations for the nonredundant set of generators can also immediately be inferred from the Pauli-principle: $\Phi^n\Phi^m = (G\partial^n G)(G\partial^m G) = -G^2(\partial^n G)(\partial^m G) = 0$. However, (6.5.5) encodes more relations. For example (6.5.5) and (6.5.3) imply $X^{0,1}\partial^2 X^{0,1} = X^{0,1}(X^{2,1} + 2X^{1,2} + X^{0,3}) = X^{0,1}X^{1,2} = -X^{0,1}X^{1,2}$. For the nonredundant set of generators this implies the following relation at scale dimension 10:

$$\Phi^1\partial^2\Phi^1 = 0. \tag{6.5.8}$$

As a simple second example we consider two commuting copies of the Virasoro algebra (L_1 and L_2) with equal central charges. Then $W := L_1 - L_2$ is primary with respect to $L := L_1 + L_2$. Furthermore, $\rho(L) = L$ and $\rho(W) = -W$ is an automorphism of this $\mathcal{W}(2, 2)$. According to (6.5.4) the subspace invariant under ρ is generated by the following fields:

$$L, \qquad \tilde{\Phi}^n := W\partial^n W \qquad \text{for all even } n. \tag{6.5.9}$$

Again, we obtain one generator at each positive even scale dimension. In this case rewriting the relations (6.5.5) for the redundant set (6.5.3) in terms of the nonredundant set (6.5.4) is slightly more complicated. Using the notation $X^{i,j} = W^{(i)}W^{(j)}$ one checks that from (6.5.3) and (6.5.5a) $\partial^2(X^{0,0}X^{0,0}) = 8X^{0,1}X^{0,1} + 2X^{0,0}\partial^2 X^{0,0}$ and $\partial^2 X^{0,0} = 2X^{1,1} + 2X^{0,2}$. Using (6.5.5b) it is straightforward to check that $\partial^2(X^{0,0}X^{0,0}) + 6X^{0,0}\partial^2 X^{0,0} + 8X^{0,0}X^{0,2} = 0$. This relation arises at scale dimension 10, which is the lowest scale dimension admitting a relation. In terms of the generators (6.5.9) it reads

$$\partial^2(\tilde{\Phi}^0\tilde{\Phi}^0) - 6\tilde{\Phi}^0\partial^2\tilde{\Phi}^0 + 8\tilde{\Phi}^0\tilde{\Phi}^2 = 0. \tag{6.5.10}$$

Now we turn to a discussion of cosets. First, we briefly discuss cosets of the type $W/\mathcal{G}$ with $\mathcal{G}$ as simple Lie algebra. By definition, the generating set of the coset is a generating set for those differential polynomials in W that are invariant with respect to the action of $\mathcal{G}$. Problems of this type are known in the mathematical literature under the name of '*invariant theory*' and one can use their results (see e.g. [124]) in order to obtain a generating set. Observing that $\hat{\mathcal{G}}_k \subset W$ and that there is always an invariant bilinear form on $\mathcal{G}$ it is immediately clear that the coset will have infinitely many generators because any bilinear expression in the currents of $\hat{\mathcal{G}}_k$ with an arbitrary number of derivatives is an invariant field. Concerning the relations one also sees that there will be infinitely many of them because non-trivial invariant polynomials in *finitely* many variables always satisfy some relations. Now one can put infinitely many derivatives (like for the generators) and it is clear that there will be infinitely many relations.

Cosets of the type $W/\hat{\mathcal{G}}_k$ are a bit more complicated. The following result was obtained in [31]: Assume that the restriction of the central term of W to $\hat{\mathcal{G}}_k$ is nondegenerate (we do note assume $\mathcal{G}$ to be simple) and that it is possible to partition the generating fields of W into the generating fields J_a of $\hat{\mathcal{G}}_k$ and a complementary set of generating fields $J_i^{\perp}$ that form primary multiplets with respect to the current algebra $\hat{\mathcal{G}}_k$ (to avoid confusion note that the $J_i^{\perp}$ need not have conformal dimension one). Under these conditions the adjoint action of $\hat{\mathcal{G}}_k$ on its complement W is a representation of $\mathcal{G}$:

$$\{J_a(z), J_i^{\perp}(w)\} = \sum_j \frac{T(a)_i^j J_j^{\perp}(w)}{(z-w)} \tag{6.5.11}$$

in terms of matrices $T(a)$. Now one introduces a covariant derivative $\mathcal{D}$ acting on the fields $J_i^{\perp}$

$$\mathcal{D}J_i^{\perp} := \partial J_i^{\perp} - \frac{1}{k}\sum_{a,b,j} J_b g^{ba} T(a)_i^j J_j^{\perp} \tag{6.5.12}$$

where g^{ba} is the inverse of the metric on $\mathcal{G}$. Note that the covariant derivative $\mathcal{D}$ is indeed a derivation. The reason simply is that if a field ϕ transforms under a representation T and χ under a representation $\hat{T}$ then $\phi\partial^n\chi$ transforms under the tensor product of the representations T and $\hat{T}$.

Now the coset $W/\hat{\mathcal{G}}_k$ is the space of those $\mathcal{G}$-invariant differential polynomials in the fields $J_i^{\perp}$ where as derivative the covariant derivative (6.5.12) has to be used. From this characterization it is immediately clear that $W/\hat{\mathcal{G}}_k$ must have infinitely many generators satisfying infinitely many constraints precisely for the same reasons as for $W/\mathcal{G}$.

A simple consequence of this general result is that for classical cosets of type $\hat{\mathcal{G}}_k \oplus \hat{\mathcal{H}}_m/\hat{\mathcal{H}}_{ik+m}$ (where i denotes the Dynkin index of the embedding $\mathcal{H} \subset \mathcal{G}$) one has

$$\lim_{m\to\infty} \frac{\hat{\mathcal{G}}_k \oplus \hat{\mathcal{H}}_m}{\hat{\mathcal{H}}_{ik+m}} = \frac{\hat{\mathcal{G}}_k}{\mathcal{H}} \tag{6.5.13}$$

and that the coset on the l.h.s. for generic m is a deformation of the coset on the r.h.s. Eq. (6.5.13) is also true for cosets of quantum $\mathcal{W}$-algebras (see e.g. [34]).

Let us now conclude this general discussion of classical cosets and turn to some more concrete statements. First we observe that if one wants to perform quasi-primary projections in coset $\mathcal{W}$-algebras one may use the formula (6.4.6) if one replaces the ordinary derivative ∂ by the covariant derivative $\mathcal{D}$. The reason is mainly that $\mathcal{D} - \partial$ commutes with the coset energy-momentum tensor L.

For cosets of Kac-Moody algebras the coset energy-momentum tensor L is always composite which implies $c = 0$. Then L is obviously primary. Under these conditions the following fields are primary as well if ϕ and χ are primary fields of dimension $d(\phi)$ and $d(\chi)$ respectively:

$$\mathcal{Q}^{(0)}(\phi, \chi) = \phi\chi\,, \qquad \tfrac{1}{2}\mathcal{Q}^{(1)}(\phi, \chi) = d(\phi)\phi\chi' - d(\chi)\phi'\chi\,. \tag{6.5.14}$$

As a curiosity aside we note that the covariance properties of the second expression have already been noted several decades ago in a different context (see e.g. eq. (24) on page 23 of [125]). It should be clear to the reader that the assumptions of claim II are not satisfied for composite L and thus there need not be a primary generating set.

Let us now illustrate these basic remarks with a few statements on some classical cosets. The absence of a primary generating set can be seen very nicely in the classical coset $\widehat{sl(2)}/\widehat{U(1)}$ (compare also [122]). The fields

$$W_{n+2} := \mathcal{Q}^{(n)}(J^+, J^-)\,, \qquad 0 \leq n \in \mathbb{Z} \tag{6.5.15}$$

form a quasi-primary generating set of the classical coset $\widehat{sl(2)}/\widehat{U(1)}$ (for the relations see [31]). The fields (6.5.15) cannot have a primary projection unless they are already primary. It can be checked explicitly that $W_2 = kL$ and W_3 are primary whereas W_4, W_5 and W_6 are *not* primary. This demonstrates that there is no primary basis in the classical coset $\widehat{sl(2)}/\widehat{U(1)}$ [7]).

Also the classical coset $SVIR(N = 2)/\widehat{U(1)}$ can be controlled quite well. One finds precisely one generator for each integer scale dimension greater or equal to two. For this coset the energy-momentum tensor L has a non-vanishing central term because it is not composite. Thus, according to claim II it should be possible to choose the generators with dimension greater than two such that they are primary. This can in fact be checked explicitly for small conformal dimensions (we have performed checks up to conformal dimension five). For more details on this coset see [31].

Finally, let us briefly consider the classical coset $\widehat{sl(2)}_k/sl(2)$. From the discussion of the $\beta - \gamma$-system in [31] one expects that the classical coset $\widehat{sl(2)}_k/sl(2)$ should have a specific Poisson subalgebra at $k = -\frac{1}{2}$. In order to check this one can perform explicit computations of Poisson brackets in $\widehat{sl(2)}_k/sl(2)$ at low scale dimension. We use normalization conventions analogous to [28]. According to [31] we have to consider the following

[7]) Note, however, that due to (6.5.14) there are more primary fields in this coset than claimed in [122].

generators:

$$\begin{aligned}
S_{m,n} &:= (\partial^m J^+)\partial^n J^- + \tfrac{1}{2}(\partial^m J^0)\partial^n J^0 + (\partial^m J^-)\partial^n J^+ \,, \\
S_{m,n,k} &:= (\partial^m J^-)(\partial^n J^0)\partial^k J^+ - (\partial^m J^-)(\partial^n J^+)\partial^k J^0 - (\partial^m J^0)(\partial^n J^-)\partial^k J^+ \\
&\quad + (\partial^m J^0)(\partial^n J^+)\partial^k J^- + (\partial^m J^+)(\partial^n J^-)\partial^k J^0 - (\partial^m J^+)(\partial^n J^0)\partial^k J^- \,.
\end{aligned} \tag{6.5.16}$$

Eliminating the redundant generators from (6.5.16) we see that this classical coset is of type $\mathcal{W}(2,4,6,6,8,8,9,10,10,\ldots)$. We can choose the following non-redundant quasi-primary generators up to scale dimension 6:

$$\begin{aligned}
L &= \tfrac{1}{2k} S_{0,0} \,, \\
W_4 &= S_{0,2} + \tfrac{3}{2} S_{1,1} \,, \\
W_{6\mathrm{a}} &= S_{0,4} - 10 S_{1,3} + 10 S_{2,2} \,, \\
W_{6\mathrm{b}} &= S_{0,1,2}.
\end{aligned} \tag{6.5.17}$$

One can check that L and $W_{6\mathrm{b}}$ are primary whereas W_4 and $W_{6\mathrm{a}}$ are only quasi-primary which once again demonstrates the absence of a primary generating set. Looking for a Poisson subring one finds the following useful linear combination of generators:

$$\hat{W}_6 := \frac{k}{7} W_{6\mathrm{a}} - 2 W_{6\mathrm{b}} \,. \tag{6.5.18}$$

We have checked up to scale dimension 6 that L, W_4 and $\hat{W}_6$ close among themselves under Poisson brackets for all k (i.e. we have not looked at any fields beyond scale dimension 6 on the r.h.s. of the classical OPEs – still a quite non-trivial fact). From this observation and the study of the $\beta-\gamma$-system in [31] it seems sensible to expect that the classical coset $\widehat{sl(2)}_k / sl(2)$ has a Poisson subalgebra generated by specific even dimensional fields for all values of the level k.

Concerning the quantum case of orbifolds and cosets in general there is the following hypothesis: Upon normal ordering of the classical relations correction terms emerge that contain classical generators such that one can eliminate precisely one generator per generator of the classical relations. This '*cancellation*' has been checked so far rigorously only for a very simple coset [31] and for a few dimensions in some other cosets and orbifolds [31, 28]. Note that the character argument which has been used in the argumentation supporting the results of the next section relies heavily on the assumption that this cancellation always happens.

6.6. The structure of quantum $\mathcal{W}$-algebras

One of the main aims of the explicit constructions of quantum $\mathcal{W}$-algebras e.g. in refs. [30, 102, 94, 51] was to gain some insight into the structure of quantum $\mathcal{W}$-algebras and the associated rational conformal field theories (RCFTs). The rational models of those $\mathcal{W}$-algebras existing for isolated c only can be either interpreted as extensions or truncations of $\mathcal{W}$-algebras obtained by DS reduction, or the effective central charge is integer (see [49] for a summary). After identifying the Casimir $\mathcal{W}$-algebras and the orbifold of the $N=1$ super Virasoro algebra among the $\mathcal{W}$-algebras existing for generic c two unexplained solutions remained: An algebra of type $\mathcal{W}(2,4,6)$ [102] and an algebra of type $\mathcal{W}(2,3,4,5)$ [94] which both give rise to generic null fields. In particular the origin of this $\mathcal{W}(2,4,6)$ was unexplained for some time [51]. In the meantime both of these algebras have been identified [31, 27, 28] and it was realized that they fit in a general new structure: They play the rôle of '*unifying $\mathcal{W}$-algebras*' for Casimir $\mathcal{W}$-algebras [27, 28]. The purpose of this section is to explain this new unifying structure.

One of the basic observations is that truncations of Casimir $\mathcal{W}$-algebras are quite general, i.e. that for certain values of the central charge c some of the generators turn out to be null fields. This can be investigated systematically using the Kac determinant [33] for the vacuum representation. This has been carried out in [27] leading to the truncations in table 8.

Casimir algebra	c	*truncated algebra*
$\mathcal{WA}_n$	$c_{\mathcal{A}_n}(n+r, n+s)$	$\mathcal{W}(2,\ldots,rs-1)$
$\mathcal{WB}_n$	$c_{\mathcal{B}_n}(2n-2+r, 2n-1+s)$	$\mathcal{W}(2,4,\ldots,rs-2)$ for $r{\cdot}s$ even
$\mathcal{WC}_n$	$c_{\mathcal{C}_n}(n+r, 2n-1+s)$	$\mathcal{W}(2,4,\ldots,rs-2)$ for $r{\cdot}s$ even
Orb $(\mathcal{WD}_n)$	$c_{\mathcal{D}_n}(2n-3+r, 2n-3+s)$	$\mathcal{W}(2,4,\ldots,rs-2)$ for $r{\cdot}s$ even

Table 8: Truncations of Casimir $\mathcal{W}$-algebras

The parameterization of the central charge in table 8 is given by the following generalization of (6.2.2):

$$c_{\mathcal{L}_n}(p,q) = n - 12\frac{(q\rho - p\rho^\vee)^2}{pq} \tag{6.6.1}$$

where $\rho^\vee$ is the dual Weyl vector (for simply laced $\mathcal{L}_n$ one has $\rho^\vee = \rho$).

The result of table 8 gives rise to the structure indicated for the Casimir $\mathcal{W}$-algebras $\mathcal{WA}_n$ in Fig. 4. The horizontal lines correspond to the algebras $\mathcal{WA}_n$ that exist for generic central charge c (or equivalently, generic 'level' k). For the kth unitary minimal model all generators of $\mathcal{WA}_n$ with dimension greater than k^2+3k+1 become null fields leading to a truncation of $\mathcal{WA}_n$ to an algebra of type $\mathcal{W}(2,\ldots,k^2+3k+1)$ for all sufficiently large n. It was argued in [27] that one can interpolate these truncations at fixed k to non-integer n giving rise to a new $\mathcal{W}$-algebra existing for generic c – a '*unifying $\mathcal{W}$-algebra*'.

In general we will call a $\mathcal{W}$-algebra a unifying $\mathcal{W}$-algebra if it is finitely generated, exists for generic c and has the property that a discrete family of $\mathcal{W}$-algebras exists (e.g. Casimir $\mathcal{W}$-algebras based on a Lie algebra of fixed type) such that infinitely many members of this family at certain distinct values of the central charge truncate to this unifying algebra. Since unifying $\mathcal{W}$-algebras exist for generic c they can e.g. be thought of as continuations of Casimir $\mathcal{W}$-algebras $\mathcal{WL}_n$ to real values of the rank n for certain values of the central charge. Usually, unifying $\mathcal{W}$-algebras give rise to null fields, i.e. they are *non-freely* generated.

The part of Fig. 4 corresponding to unitary minimal models (k a positive integer) can be understood in terms of level-rank duality [9, 34] using the coset realization of $\mathcal{WA}_{n-1}$:

$$\mathcal{WA}_{n-1} \cong \frac{\widehat{sl(n)}_k \oplus \widehat{sl(n)}_1}{\widehat{sl(n)}_{k+1}} \cong \frac{\widehat{sl(k+1)}_n}{\widehat{sl(k)}_n \oplus \widehat{U(1)}} = \mathcal{CP}(k)\,. \tag{6.6.2}$$

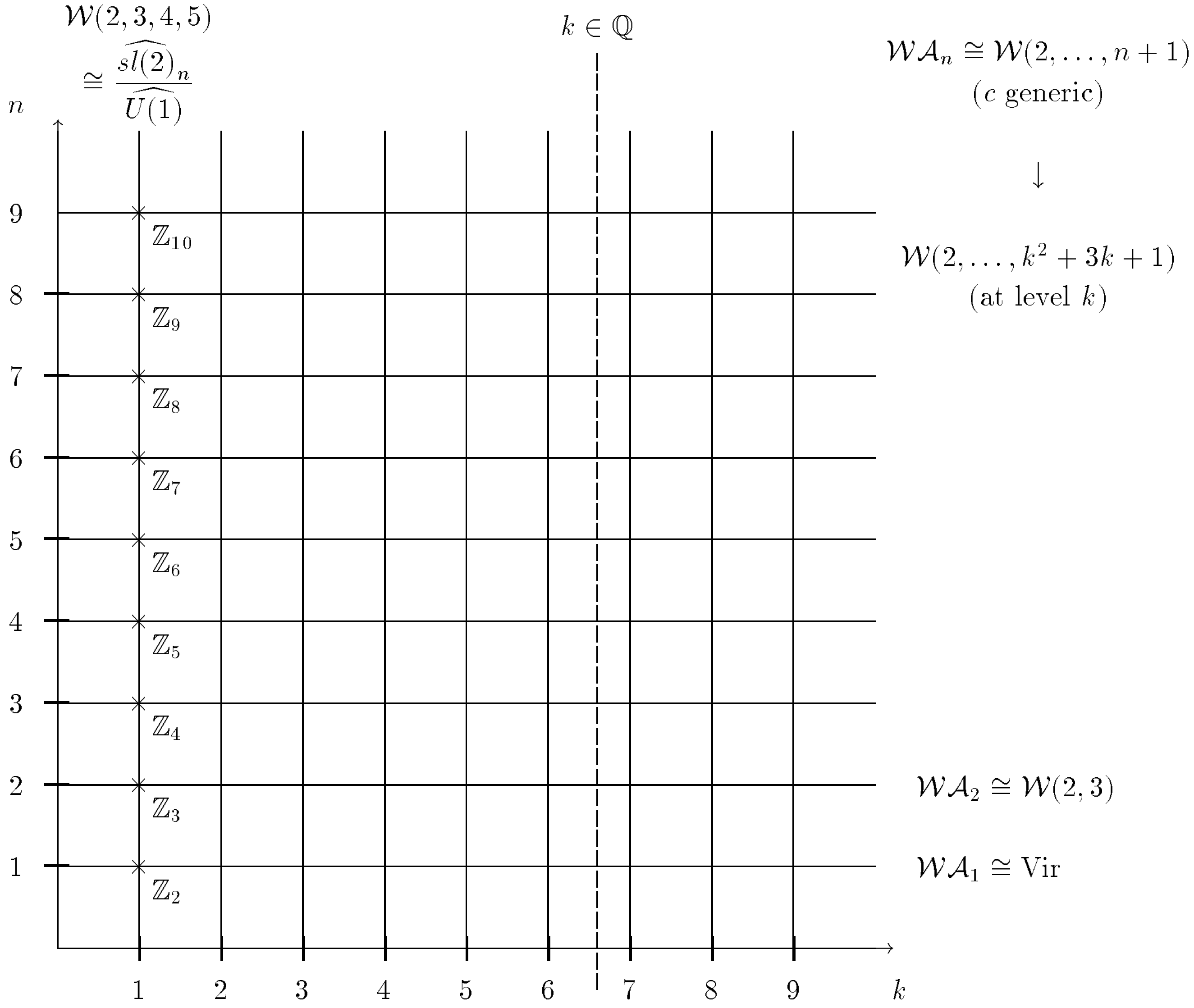

Fig. 4: The structure of the Casimir $\mathcal{W}$-algebras $\mathcal{WA}_n$ and their unifying $\mathcal{W}$-algebras.

More precisely, it was shown [9, 34] that the cosets in (6.6.2) give rise to equivalent energy-momentum tensors. In [28] evidence was collected that (6.6.2) is in fact true on the level of $\mathcal{W}$-algebras. Thus, the symmetry algebra of the $\mathcal{CP}(k)$ model is a unifying $\mathcal{W}$-algebra for the kth unitary minimal model of $\mathcal{WA}_{n-1}$. Note that the l.h.s. of (6.6.2) is defined for integer n and arbitrary k, whereas the r.h.s. is defined for integer k and general n. The isomorphism in (6.6.2) is valid iff k and n are both positive integers. Note that $\mathcal{CP}(k)$ does indeed exist for generic c or k, thus giving rise to a coset realization of the unifying $\mathcal{W}$-algebra predicted by inspection of the Kac-determinant.

It was argued in [28] that the field content of $\mathcal{CP}(k)$ is given by

$$\mathcal{CP}(k) \cong \mathcal{W}(2,3,\ldots,k^2+3k+1) \tag{6.6.3}$$

with two generic null fields at dimension k^2+3k+4 which is consistent with the prediction from the Kac-determinant.

Now we would like to discuss the first unitary minimal models of the algebras $\mathcal{WA}_{n-1}$ in some more detail. On the one hand, the case $k=1$ corresponds to the $\mathbb{Z}_n$ parafermions which are relevant to the $\mathbb{Z}_n$-quantum spin chains that we have discussed earlier. On the other hand, the coset $\widehat{sl(2)}_n/\widehat{U(1)}$ arising at $k=1$ obviously has two effective degrees of freedom, and using the character argument of P. Bouwknegt (see e.g. [33]) it is obvious that it should be finitely generated. Nevertheless, there is some confusion about this question of the generating set in the literature (see e.g. [18, 112, 127]). Therefore we would like to explicitly recall what we have been able to show with some effort in [28]:

Proposition III: *([28]) The quantum coset $\widehat{sl(2)}_n/\widehat{U(1)}$ has a closed $\mathcal{W}(2,3,4,5)$ subalgebra with two generic null fields at conformal dimension 8. Furthermore, there are no additional generators of conformal dimension 6, 7 or 8 in the coset $\widehat{sl(2)}_n/\widehat{U(1)}$.* ■

Remarks:

1) More strongly, a character argument [28] indicates that the coset $\widehat{sl(2)}_n/\widehat{U(1)}$ is isomorphic to the $\mathcal{W}(2,3,4,5)$. Unfortunately, we have not been able to prove this stronger statement.
2) This $\mathcal{W}(2,3,4,5)$ is the previously unexplained algebra found in [94].

We have already mentioned that this $\mathcal{W}(2,3,4,5)$ unifies the first unitary minimal models of $\mathcal{WA}_{n-1}$ that are related to critical points in the $\mathbb{Z}_n$-spin quantum chains of earlier sections. In view of sections 6.2 and 6.3 we would be interested in the twisted sector of this algebra. Indeed, an inner automorphism of $\widehat{sl(2)}_n$ gives rise to an outer $\mathbb{Z}_2$ automorphism of the coset $\widehat{sl(2)}_n/\widehat{U(1)}$ [28]. Unfortunately, at the moment we do not know how to apply the standard machinery of coset representations in the presence of an inner automorphism which means that in contrast to the periodic sector the twisted sector cannot be easily obtained from the coset construction. Nevertheless, one can argue that the orbifold is of type $\mathcal{W}(2,4,6,8,10)$ with a generic null field at scale dimension 14 for generic n. According to section 6.3 this orbifold should be relevant for the $\mathbb{Z}_n$-spin chain with *free* boundary conditions. We conclude this discussion by recalling the simple observation that due to the coset realization the irreducible modules of $\mathbb{Z}_n$ parafermionic model can grow at most as fast as a free module of two chiral bosonic fields. It would be interesting to see if the presence of a unifying object at generic real n can be used for obtaining more insights into $\mathbb{Z}_n$ parafermionic conformal field theories.

The investigation of the Kac determinant is not restricted to integer k but also applies to $k \in \mathbb{Q}$ – including in particular the non-unitary minimal models. Using the parameterization (6.6.1) the field content can be read off from table 8. As before, one can interpolate these further unifying $\mathcal{W}$-algebras to generic n (or c). These unifying $\mathcal{W}$-algebras can also be realized in terms of cosets. Now, one needs Drinfeld-Sokolov reductions based on $sl(r)$ for a *non-principal* embedding such that they have a $\widehat{sl(k)} \oplus \widehat{U(1)}$ Kac-Moody subalgebra:

$$\mathcal{W}^{sl(r)}_{r-k,1^k} = \mathcal{W}(1^{k^2}, 2, 3, \ldots, r-k, \left(\tfrac{r-k+1}{2}\right)^{2k}). \tag{6.6.4}$$

The k^2 currents form a $\widehat{sl(k)} \oplus \widehat{U(1)}$ Kac-Moody algebra, the fields of dimension 2, ..., $r-k$ are singlets with respect to this Kac-Moody and the $2k$ fields of dimension $\frac{r-k+1}{2}$ are a Kac-Moody multiplet. More precisely, these $2k$ fields transform as two $U(1)$-charge conjugate defining representations of $sl(k)$. In [28] it was argued that

$$\mathcal{WA}_{n-1} \cong \frac{\mathcal{W}^{sl(r)}_{r-k,1^k}}{\widehat{sl(k)} \oplus \widehat{U(1)}} \cong \mathcal{W}(2, 3, \ldots, (k+1)r+k) \qquad \text{at} \qquad c_{\mathcal{A}_{n-1}}(n+k, n+r) \tag{6.6.5}$$

with two generic null fields at dimension $(k+1)r+k+3$. Identifying $\mathcal{W}^{sl(r+1)}_{1^{r+1}}$ with the unconstrained $\widehat{sl(r+1)}$ Kac-Moody algebra, the case $r = k+1$ is identical to the $\mathcal{CP}(k)$ cosets which we have already discussed. One can also apply (6.6.5) to the case $k = 0$. In this case, the $sl(2)$ embedding is the principal one and there is no Kac-Moody subalgebra. Thus, the coset in (6.6.5) is just $\mathcal{WA}_{r-1}$ and we recover eq. (2.4) of ref. [27] (note that this equality was originally observed in [106]).

The Casimir algebras $\mathcal{WA}_n$ in Fig. 4 obviously exist also for negative k and from the preceding discussion we conclude that one can make sense of the unifying $\mathcal{W}$-algebras also for negative n. However, it is also possible to directly make sense of $\mathcal{WA}_n$ at negative n [96] (compare also the comments on $\mathcal{WD}_{-m}$ below) or even for complex $n \in \mathbb{C}$ [53]. Among those, the $\mathcal{WA}_n$ at negative n are defined less formally since they can be given a coset realization $\mathcal{WA}_{-n-1} \cong (\widehat{sl(n)}_k \oplus \widehat{sl(n)}_{-1})/\widehat{sl(n)}_{k-1}$ and have a definite finite generating set [96].

Using $\mathcal{WA}_n$ for real n or the fact that Fig. 4 is densely covered by unifying $\mathcal{W}$-algebras one can define [96] a '*universal*' $\mathcal{W}$-algebra for all Casimir algebra based on $\mathcal{A}_n$ that depends on *two* parameters, e.g. k and n. For generic irrational $k \notin \mathbb{Q}$ this universal $\mathcal{W}$-algebra will have infinitely many generators. Doing so, one can nicely fit the $\mathcal{W}_\infty$ and $\mathcal{W}_{1+\infty}$ algebras (see e.g. [17]) in the picture of Fig. 4: They can be recovered from the topmost border $n = \infty$ respective right border $k = \infty$. Then, e.g. the truncations of $\mathcal{W}_{1+\infty}$ at $c = n$ [64] arise naturally from Fig. 4 (for more details see [28]).

To summarize, the picture of the space of all Casimir algebras $\mathcal{WA}_n$ and their unifying $\mathcal{W}$-algebras as presented in Fig. 4 is mainly a conjecture. However, this conjecture has been thoroughly checked in [27, 28]: Beyond the inspection of the Kac determinant and cross-checks with limiting cases which we mentioned above one can perform character computations for the cosets and compare structure constants or minimal models (where known). Even more, the simplest of the relevant cosets can be constructed explicitly [28] and e.g. the statement about the generating set can be quite rigorously verified.

The structure of the Casimir algebras $\mathcal{WD}_n$, $\mathcal{WC}_n$ and $\mathcal{WB}_n$ is similar to Fig. 4 which we have discussed in some detail. The truncations inferred from the Kac determinant are presented in table 8. Whereas in the case of $\mathcal{WA}_n$ we were able to provide a coset realization for all unifying $\mathcal{W}$-algebras, coset realizations of unifying $\mathcal{W}$-algebras for the other Casimir algebras are only partially known. The known coset realizations for unifying $\mathcal{W}$-algebras of Casimir algebras are summarized in table 9 (for a detailed discussion see [28]). Sometimes an additional $\mathbb{Z}_2$ orbifold is needed which is denoted by 'Orb' in table 9. If 'Orb' is put in brackets only part of the algebras give rise to non-trivial outer automorphisms – for the other ones we do not have to take an orbifold.

Casimir algebra	*central charge* c	*coset realization of unifying algebra*	*dimensions of simple fields*	*dimension of first null field*
$\mathcal{WA}_{n-1}$	$c_{\mathcal{A}_{n-1}}(n{+}k, n{+}r)$	$\frac{\mathcal{W}^{sl(r)}_{r-k,1^k}}{\widehat{sl(k)}\oplus \widehat{U(1)}}$	$2,3,\ldots,kr+r+k$	$kr+r+k+3$
$\mathcal{WB}_n$	$c_{\mathcal{B}_n}(2n{+}k{-}1, 2n{+}1)$ $c_{\mathcal{B}_n}(2n, 2n{+}k)$	$(\mathrm{Orb})\left(\frac{\widehat{so(k)}_\kappa \oplus \widehat{so(k)}_1}{\widehat{so(k)}_{\kappa+1}}\right)$	$2,4,\ldots,2k$	$2k+4$
$\mathcal{WC}_n$	$c_{\mathcal{C}_n}(n{+}k{+}1, 2n{+}2k{+}1)$	$\frac{\widehat{sp(2k)}_n \oplus \widehat{sp(2k)}_{-\frac{1}{2}}}{\widehat{sp(2k)}_{n-\frac{1}{2}}}$	$2,4,\ldots,2k^2+4k$	$2k^2+4k+5$
$\mathrm{Orb}\,(\mathcal{WD}_n)$	$c_{\mathcal{D}_n}(2n{+}k{-}2, 2n{+}k{-}1)$	$\mathrm{Orb}\left(\frac{\widehat{so(k+1)}_{2n}}{\widehat{so(k)}_{2n}}\right)$	$2,4,\ldots,k^2+3k$	k^2+3k+4

Table 9: Coset realizations of unifying $\mathcal{W}$-algebras

Among the unifying $\mathcal{W}$-algebras for these three families of Casimir algebras those for $\mathcal{WC}_n$ are particularly interesting because they can in some sense be regarded as algebras of type '$\mathcal{WD}_{-k}$' – continuations of the $\mathcal{WD}_m$ series of Casimir algebras to negative m. Historically, the mysterious $\mathcal{W}(2,4,6)$ was the starting point for the discovery of unifying $\mathcal{W}$-algebras in [27, 28]. It was proposed in [95] that this $\mathcal{W}(2,4,6)$ can in some sense be regarded as belonging to the series of $\mathcal{WD}_n$ Casimir algebras: $\mathcal{W}(2,4,6) \cong \mathcal{WD}_{-1}$. Furthermore, all known minimal models of this $\mathcal{W}(2,4,6)$ [51] were identical with minimal models of some $\mathcal{WC}_n$ Casimir algebra. Only after generalizing these observations we became aware that the algebras $\mathcal{WD}_{-k}$ can be given a group theoretical meaning.

Negative dimensional groups are known in the literature (see e.g. [46]). More precisely, some aspects of the representation theory of the classical groups can be understood naturally after continuation to negative dimensions. For example, the dimension formulas for $SO(2n)$ and $Sp(2m)$ can be related by transposition of the Young tableaux for $m = -n$. Similar relations can also be established for the Casimir operators upon interchanging symmetrization and antisymmetrization. These observations can be written in a compact form e.g. $SO(-2n) \cong \overline{Sp(2n)}$ where the overbar means interchange of symmetrization and antisymmetrization. For the Kac-Moody algebras one can now establish a relation for the levels by equating the central charges of the Sugawara energy-momentum tensors. For the case we are interested in one finds [28]:

$$\widehat{so(-2k)}_\kappa = \widehat{sp(2k)}_{-\frac{\kappa}{2}}\,. \tag{6.6.6}$$

Thus, from the coset realization of $\mathcal{WD}_m$ one finds that

$$\mathcal{WD}_{-k} \cong \frac{\widehat{sp(2k)}_\kappa \otimes \widehat{sp(2k)}_{-\frac{1}{2}}}{\widehat{sp(2k)}_{\kappa-\frac{1}{2}}} \cong \mathcal{W}(2,4,\dots,2k(k+2)) \tag{6.6.7}$$

with a first generic null field at conformal dimension $2k^2+4k+5$. This fields content can e.g. be inferred from a character argument [28]. The algebras $\mathcal{WD}_{-k}$ are also supposed to be unifying $\mathcal{W}$-algebras for the $\mathcal{WC}_n$ Casimir algebras [27]:

$$\mathcal{WD}_{-k} \cong \mathcal{WC}_n \qquad \text{at} \qquad c_{\mathcal{C}_n}(n+k+1, 2n+2k+1)\,. \tag{6.6.8}$$

The field content of (6.6.7) is consistent with the truncations of table 8 predicted for the minimal models of (6.6.8).

To summarize, the space of all $\mathcal{W}$-algebras gives rise to complicated structures including a '*unifying structure*' that we have discussed in this section. However, there are indications [28] that the only rational models of unifying $\mathcal{W}$-algebras are located at intersection points with the Casimir $\mathcal{W}$-algebras. This implies that unifying $\mathcal{W}$-algebras do probably not give rise to new RCFTs, and that the classification problem of RCFTs (which is far from being solved) might in fact be simpler than a classification of $\mathcal{W}$-algebras. One might hope that (super-symmetric) quantized DS exhausts all possible RCFTs (with exceptions at (half-)integer effective central charge). Thus, it would be desirable to have at least a good understanding of representations of *non-principal* DS $\mathcal{W}$-algebras where very little is known so far. Nevertheless, the unifying $\mathcal{W}$-algebras could still be of some use because on the one hand they might lead to conceptual simplifications and on the other hand not all physical phenomena are necessarily described by RCFTs.

... In these colleges, the professors contrive new rules and methods of agriculture and building, and new instruments and tools for all trades and manufactures, whereby, as they undertake, one man shall do the work of ten; a palace may be built in a week, of materials so durable as to last forever without repairing. All the fruits of the earth shall come to maturity at whatever season we think fit to choose, and increase an hundred-fold more than they do at present; with innumerable other happy proposals. The only inconvenience is, that none of these projects are yet brought to perfection; ...

Jonathan Swift in "A Voyage to Balnibarbi"

7. Conclusion

In this thesis we have discussed several aspects of quantum spin models and extended conformal algebras.

We have investigated an algebraic condition that guarantees integrability of quantum spin models – the so-called 'Dolan-Grady-condition' (also called superintegrability). In one dimension we achieved a classification of superintegrable nearest neighbour interaction quantum spin models based on $sl(2)$. For two dimensions the only result we obtained so far is a non-existence statement of certain superintegrable spin-1/2 models. Nevertheless, this approach seems to be feasible also in higher dimensions and deserves further attention.

In a large part of this thesis we have studied the $\mathbb{Z}_n$-chiral Potts model without necessarily demanding integrability. We have presented an argument using perturbation theory that shows that the massive high-temperature phases of all $\mathbb{Z}_n$-spin quantum chains exhibit quasiparticle spectra with $n-1$ fundamental particles. Since the argument relies on perturbation theory it applies rigorously only to very high temperatures. Due to the perturbative nature of the details we were not able to give it any predictive power for those case where some of the fundamental particles cross with scattering states. For these cases one needs different methods, e.g. Bethe ansatz techniques [41, 103] or numerical methods [69]. Nevertheless, the basic idea of approximating a multi-particle state by single-particle states sitting on subparts of the chain might be applicable in the entire massive high-temperature phase.
Our derivation of the quasiparticle picture involving $n-1$ fundamental particles is valid also for the scaling region near the conformal point $\lambda = 1$, $\phi = \varphi = 0$, the only non-rigorous part of the proof being the radius of convergence.

Having derived such a quasiparticle picture the main open problem to obtain the scattering matrix of the corresponding massive field theory.

Furthermore, we discussed a general duality property stating equality of spectra in the low- and high-temperature phase. Thus, the quasiparticle interpretation for the high-temperature phase of the general $\mathbb{Z}_n$-chiral Potts quantum chain can be pulled over to the low-temperature phase. However, charge Q and boundary conditions R are interchanged by the duality transformation. In particular, for periodic boundary conditions one sees only energy levels above the ground state that correspond to composite particle states.

We also studied correlation functions using a perturbation expansion for the ground state of the $\mathbb{Z}_3$-model and numerical techniques. Although these approaches are limited to short ranges, we were not only able to estimate correlation lengths in the massive high-temperature phase but it also turned out that the correlation functions have oscillatory contributions. For very high temperatures the oscillation length is proportional to the inverse of one of the chiral angles $L \sim \phi^{-1}$. We further observed that the oscillation length is closely related to the minimum of the dispersion relations for general values of the parameters. The relation $LP_{\text{min}} = 2\pi$ is valid on the lattice with a much better accuracy than the well-known relation $\xi \sim m^{-1}$. For special values of the parameters we were able to derive the relation $LP_{\text{min}} = 2\pi$ from a form factor decomposition but one should certainly try to gain more insight into the correlation functions, in particular into the long-distance behaviour of the amplitude.

We have then turned to extended conformal algebras. First, we have shown how automorphisms of $\mathcal{W}$-algebras can be used to enlarge minimal models by imposing twisted boundary conditions on the chiral fields. Some of these rational conformal fields theories are relevant for the $\mathbb{Z}_n$-spin quantum chains. Furthermore, there is a striking one-to-one correspondence of boundary conditions for the chiral fields of a $\mathcal{W}$-algebra and the quantum spin chain.

Classical $\mathcal{W}$-algebras are an ideal testing ground for the study of construction principles. Surprisingly, certain basic properties can not as easily be derived for them as for quantum $\mathcal{W}$-algebras. We have argued that the space of fields of a classical $\mathcal{W}$-algebra should under very general conditions decompose into $su(1,1)$ highest weight representations, i.e. it should admit a basis of quasi-primary fields and derivatives thereof. We have also explained why we expect that it should be possible to choose the generators primary for a classical $\mathcal{W}$-algebra if, in addition, the conformal dimensions of all generators are strictly positive and the Virasoro centre c is non-zero.

Classical cosets and orbifolds can be treated systematically. For orbifolds with respect to a $\mathbb{Z}_2$ automorphism the generators and relations are completely under control. Concerning classical cosets one can in general reduce the problem of finding the generators and relations to a problem in the invariant theory of finite-dimensional Lie algebra. Where the solution to the problem in invariant theory is known (e.g. for $sl(2)$ – see [124]) the space of fields is also completely under control. It follows from general considerations that the space of fields of classical cosets and orbifolds is always an infinitely generated differential polynomial ring subject to infinitely many relations.

The situation is contrary for quantum $\mathcal{W}$-algebras. It seems that on the quantum level cosets and orbifolds are always *finitely* generated. This difference is due to a cancellation mechanism between classical generators and relations. Note however that this mechanism has been rigorously checked only for a few cases [31, 28]. Nevertheless, there had been some puzzles concerning the space of $\mathcal{W}$-algebras that could be explained once this difference was recognized.

A further difference between classical and quantum $\mathcal{W}$-algebras is that quantum $\mathcal{W}$-algebras can truncate at certain values of the central charge because some of the generators become null fields. One can argue by inspection of the Kac determinant that such truncations are in fact a very general phenomenon for quantum Casimir $\mathcal{W}$-algebras. These truncations give rise to new 'unifying' quantum $\mathcal{W}$-algebras that interpolate these truncations of Casimir $\mathcal{W}$-algebras. The notion of 'unifying $\mathcal{W}$-algebras' is a generalization and more precise version of level-rank-duality. Unifying $\mathcal{W}$-algebras can frequently be realized in terms of cosets, not only but also if this is expected from level-rank-duality. In the coset realization of unifying $\mathcal{W}$-algebras non-principal DS reductions and also negative dimensional groups play a certain rôle. In particular, algebras of type $\mathcal{WD}_{-k}$ arise as unifying $\mathcal{W}$-algebras for the Casimir algebras $\mathcal{WC}_n$.

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Appendix A: Perturbation expansions for two-particle states

In this appendix we explicitly diagonalize the first order of the perturbation expansion for two identical particles.

Let us first consider $Q_1 \neq Q_2$. In this case we specialize to $n = 3$ such that we can choose $Q_1 = 1$, $Q_2 = 2$. Now, the potential V acts in the space (4.2.9) as:

$$
\begin{aligned}
qr(V)\|t_1^{1,2}\rangle\!\rangle_P &= -\frac{2}{\sqrt{3}}\left(e^{-i(\frac{\phi}{3}-P)}\|t_{N-1}^{1,2}\rangle\!\rangle_P + 2\cos\left(\tfrac{P}{2}\right)e^{-i(\frac{\phi}{3}+\frac{P}{2})}\|t_2^{1,2}\rangle\!\rangle_P\right)\\
qr(V)\|t_j^{1,2}\rangle\!\rangle_P &= -\frac{2}{\sqrt{3}}\left(2\cos\left(\tfrac{P}{2}\right)e^{i(\frac{\phi}{3}+\frac{P}{2})}\|t_{j-1}^{1,2}\rangle\!\rangle_P + 2\cos\left(\tfrac{P}{2}\right)e^{-i(\frac{\phi}{3}+\frac{P}{2})}\|t_{j+1}^{1,2}\rangle\!\rangle_P\right)\\
&\qquad\qquad\qquad\qquad\qquad\qquad 1 < j < N-1\\
qr(V)\|t_{N-1}^{1,2}\rangle\!\rangle_P &= -\frac{2}{\sqrt{3}}\left(2\cos\left(\tfrac{P}{2}\right)e^{i(\frac{\phi}{3}+\frac{P}{2})}\|t_{N-2}^{1,2}\rangle\!\rangle_P + e^{i(\frac{\phi}{3}-P)}\|t_1^{1,2}\rangle\!\rangle_P\right)
\end{aligned}
\tag{A.1}
$$

where q is the projector onto the space (4.2.9). Although it is not difficult to diagonalize (A.1) numerically for comparably long chains (e.g. $N = 100$), we did not succeed in obtaining a closed expression for the eigenvalues or eigenvectors.

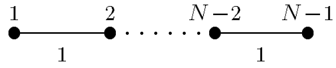
In the second case, i.e. $Q := Q_1 = Q_2$ introduce the abbreviation W by:

$$
-\frac{2}{\sin\left(\frac{\pi Q}{n}\right)}\cos\left(\frac{P}{2} - P_{\min,Q}\right)W\|t_j^{Q,Q}\rangle\!\rangle_P := qr(V)\|t_j^{Q,Q}\rangle\!\rangle_P. \tag{A.2}
$$

In the case of two identical excitations we will also have to distinguish between even and odd momenta in terms of lattice sites which is conveniently encoded in the abbreviation δ_P^N defined by (4.2.10). The action of the potential V now is

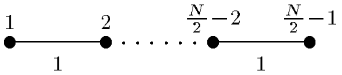
$$
\begin{aligned}
W\|t_1^{Q,Q}\rangle\!\rangle_P &= \left(e^{-i\frac{P}{2}}\|t_2^{Q,Q}\rangle\!\rangle_P\right)\\
W\|t_j^{Q,Q}\rangle\!\rangle_P &= \left(e^{i\frac{P}{2}}\|t_{j-1}^{Q,Q}\rangle\!\rangle_P + e^{-i\frac{P}{2}}\|t_{j+1}^{Q,Q}\rangle\!\rangle_P\right) \qquad 1 < j < \left[\tfrac{N}{2}\right]-1\\
W\|t_{[\frac{N}{2}]-1}^{Q,Q}\rangle\!\rangle_P &= \begin{cases} \left(e^{i\frac{P}{2}}\|t_{\frac{N-5}{2}}^{Q,Q}\rangle\!\rangle_P + e^{-i\frac{P}{2}}\|t_{\frac{N-1}{2}}^{Q,Q}\rangle\!\rangle_P\right), & \text{if } N \text{ odd;}\\ \left(e^{i\frac{P}{2}}\|t_{\frac{N}{2}-2}^{Q,Q}\rangle\!\rangle_P + \delta_P^N\sqrt{2}e^{-i\frac{P}{2}}\|t_{\frac{N}{2}}^{Q,Q}\rangle\!\rangle_P\right), & \text{if } N \text{ even}\end{cases}\\
W\|t_{[\frac{N}{2}]}^{Q,Q}\rangle\!\rangle_P &= \begin{cases} \left(e^{i\frac{P}{2}}\|t_{\frac{N-3}{2}}^{Q,Q}\rangle\!\rangle_P - (-1)^{\delta_P^N}\|t_{\frac{N-1}{2}}^{Q,Q}\rangle\!\rangle_P\right), & \text{if } N \text{ odd;}\\ \delta_P^N\sqrt{2}e^{i\frac{P}{2}}\|t_{\frac{N}{2}-1}^{Q,Q}\rangle\!\rangle_P, & \text{if } N \text{ even.}\end{cases}
\end{aligned}
\tag{A.3}
$$

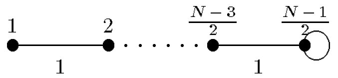
At first sight (A.3) looks much more complicated than (A.1). This is however misleading and the matrix W can be diagonalized explicitly. In order to do so, we exploit a connection to graph theory (see e.g. [80]). Before performing an explicit diagonalization we first present a graphical representation of (A.1) and (A.3). Each vector $\|t_j^{Q_1,Q_2}\rangle\!\rangle_P$ will be symbolized as a '•' with the index written above. The action of the potential V is symbolized by lines, with the square of the matrix elements (up to an isomorphism to be presented below) attached to them. Assume first that we could distinguish the two flips we make. Then the graphical representation for the action of the potential V (or W) would be

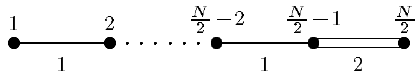


$$= (\mathcal{A}_{N-1})\,. \tag{A.4}$$

Here '$(\mathcal{L}_k)$' denotes the incidence matrix derived from the Cartan matrix of a Lie algebra $\mathcal{L}_k$. However, the states $\|t_j^{Q,Q}\rangle\rangle_P$ and $\|t_{N-j}^{Q,Q}\rangle\rangle_P$ are proportional to each other and must therefore be identified. Furthermore, it turns out that for N even and $\frac{NP}{2\pi}$ odd $\|t_{\frac{N}{2}}^{Q,Q}\rangle\rangle_P = 0$ vanishes identically. This already splits the graph (A.4) into two disjoint parts. Therefore, a graphical representation of (A.3) is given by:

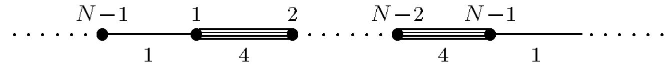
$W \cong$  $= \left(\mathcal{A}_{\frac{N}{2}-1}\right)$ for N even, $\dfrac{NP}{2\pi}$ odd

$W \cong$  $= \left(\mathcal{T}_{\frac{N-1}{2}}\right)$ for N odd (A.5)

$W \cong$  $= \left(\mathcal{B}_{\frac{N}{2}}\right)$ for N even, $\dfrac{NP}{2\pi}$ even.

Fortunately, all the graphs (A.5) have norm less or equal to 2 [8]). Because the eigenvalues of such graphs are classified [80] we can derive the first order explicitly.

In the case of (A.1) the situation is different. In order to simplify the discussion consider the case $P = \phi = 0$. Then one can represent (A.1) as

$V \approx$  . (A.6)

Note that instead of drawing a closed diagram we have represented part of it twice. It is easy to see that the norm of (A.6) is larger than 3 (it tends to 4 for $N \to \infty$). The absence of explicit expressions for the eigenvalues of such graphs prevented us from deriving an explicit expression for the first order of two-particle states in the $Q = 0$ sector even for the $\mathbb{Z}_3$-chain.

Let us now explicitly diagonalize the matrix (A.3). Although this can be done for all four different cases simultaneously it is more illustrative to treat first one case separately. The simplest case is actually N even and $\frac{NP}{2\pi}$ odd. First, we perform the following diagonal change of bases

$$B\|t_j^{Q,Q}\rangle\rangle_P := e^{-i\frac{P}{2}(j-1)}\|t_j^{Q,Q}\rangle\rangle_P\,. \tag{A.7}$$

If we also identify the $\|t_j^{Q,Q}\rangle\rangle_P$ with the standard basis of $\mathbb{C}^{\frac{N}{2}-1}$ the $\frac{N}{2}-1$ times $\frac{N}{2}-1$ matrix W satisfies

$$W = B \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix} B^{-1}. \tag{A.8}$$

[8]) $(\mathcal{T}_k)$ is the Tadpole graph.

The eigenvalues and eigenvectors of the matrix on the r.h.s. of (A.8) are well-known in the literature (see e.g. [80], example 1.2.5). We can use them to write down immediately the eigenvalues and eigenvectors of the matrix W:

$$\begin{aligned} \|\tau_k^{Q,Q}\rangle\rangle_P &:= B\frac{2}{\sqrt{N}}\begin{pmatrix} \sin\left(\frac{2k\pi}{N}\right) \\ \sin\left(\frac{2k2\pi}{N}\right) \\ \vdots \\ \sin\left(\frac{2k(\frac{N}{2}-1)\pi}{N}\right) \end{pmatrix}, \\ W\|\tau_k^{Q,Q}\rangle\rangle_P &= 2\cos\left(\frac{2k\pi}{N}\right)\|\tau_k^{Q,Q}\rangle\rangle_P\ , \qquad 1 \leq k \leq \frac{N}{2}-1. \end{aligned} \tag{A.9}$$

Putting things together one obtains the first order expansions (4.2.11) and (4.2.12) for $4 \leq N$ even, $\frac{NP}{2\pi}$ odd.

The same argument can be applied to the remaining cases. The only additional consideration is that we need a second change of bases M in $\mathbb{C}^{N-1}$. For N odd it is defined by

$$M := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & \cdots & \cdots & 0 & 1 \\ 0 & \ddots & \ddots & \iddots & \iddots & 0 \\ \vdots & \ddots & 1 & 1 & \iddots & \vdots \\ \vdots & \iddots & -1 & 1 & \ddots & \vdots \\ 0 & \iddots & \iddots & \ddots & \ddots & 0 \\ -1 & 0 & \cdots & \cdots & 0 & 1 \end{pmatrix} \qquad N-1\times N-1, N \text{ odd} \tag{A.10a}$$

whereas for N even it is defined as follows

$$M := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 & 1 \\ 0 & \ddots & \ddots & & \iddots & \iddots & 0 \\ \vdots & \ddots & 1 & 0 & 1 & \iddots & \vdots \\ \vdots & & 0 & \sqrt{2} & 0 & & \vdots \\ \vdots & \iddots & -1 & 0 & 1 & \ddots & \vdots \\ 0 & \iddots & \iddots & & \ddots & \ddots & 0 \\ -1 & 0 & \cdots & \cdots & \cdots & 0 & 1 \end{pmatrix} \qquad N-1\times N-1, N \text{ even}. \tag{A.10b}$$

With the definition (A.7) of the $N-1\times N-1$ matrix B we can write W as

$$\begin{pmatrix} W^{\text{even}} & 0 \\ 0 & W^{\text{odd}} \end{pmatrix} = BM\begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix} M^{-1}B^{-1} \tag{A.11}$$

where W^{even} is the $[\frac{N}{2}]\times[\frac{N}{2}]$ matrix W for even lattice momenta ($\delta_P^N=1$) and W^{odd} is the $[\frac{N-1}{2}]\times[\frac{N-1}{2}]$ matrix W for odd lattice momenta (with reversed order of basis vectors).

Again, we can use the well-known results [80] to write down the eigenvalues and eigenvectors of the matrix W:

$$\begin{aligned}
\|\tau_k^{Q,Q}\rangle\!\rangle_P &:= B\frac{2}{\sqrt{N}}\begin{pmatrix} \sin\left(\frac{(2k-\delta_P^N)\pi}{N}\right) \\ \sin\left(\frac{(2k-\delta_P^N)2\pi}{N}\right) \\ \vdots \\ \sin\left(\frac{(2k-\delta_P^N)([\frac{N}{2}]-1)\pi}{N}\right) \\ \sin\left(\frac{(2k-\delta_P^N)[\frac{N}{2}]\pi}{N}\right)\begin{cases}\frac{1}{\sqrt{2}} & \text{for } N \text{ even} \\ 1 & \text{for } N \text{ odd}\end{cases}\end{pmatrix}, \\
W\|\tau_k^{Q,Q}\rangle\!\rangle_P &= 2\cos\left(\frac{(2k-\delta_P^N)\pi}{N}\right)\|\tau_k^{Q,Q}\rangle\!\rangle_P\,, \qquad 1\le k\le\left[\frac{N}{2}\right].
\end{aligned} \tag{A.12}$$

Inserting definitions one immediately obtains the final results (4.2.11) and (4.2.12) from (A.12).

Let us now turn to the second order. For simplicity we restrict to the $Q=2$-sector for $n=3$ and odd N. We abbreviate the resolvent by g and its values by:

$$R_{3,1}:=-4\sqrt{3}\cos\left(\frac{\varphi}{3}\right), \qquad R_{1,2}:=-4\sqrt{3}\cos\left(\frac{\pi-\varphi}{3}\right), \qquad R_{0,1}:=4\sqrt{3}\cos\left(\frac{\pi+\varphi}{3}\right). \tag{A.13}$$

Then we obtain for the matrix elements between the states $\|t_k^{1,1}\rangle\!\rangle_P$ of the second order expression:

$$\begin{aligned}
B^{-1}\,q\,r(V)\,g\,r(V)\,q\,B = \frac{8}{3}\Bigg\{&\left[\frac{\cos\left(P-\frac{2\phi}{3}\right)+1}{R_{0,1}}-\frac{1}{R_{1,2}}+\frac{1}{R_{3,1}}\right]\begin{pmatrix}1&0&\cdots&0\\0&0&\cdots&0\\\vdots&\vdots&\ddots&\vdots\\0&0&\cdots&0\end{pmatrix} \\
&+\frac{\cos\left(\frac{P}{2}+\frac{2\phi}{3}\right)}{R_{1,2}}\begin{pmatrix}0&1&0&\cdots&0\\1&0&1&\ddots&\vdots\\0&1&\ddots&\ddots&0\\\vdots&\ddots&\ddots&0&1\\0&\cdots&0&1&0\end{pmatrix}+\frac{\cos\left(P-\frac{2\phi}{3}\right)}{R_{3,1}}\begin{pmatrix}0&0&1&\cdots&0\\0&0&0&\ddots&\vdots\\1&0&\ddots&\ddots&1\\\vdots&\ddots&\ddots&0&1\\0&\cdots&1&1&0\end{pmatrix} \\
&+\left[\frac{2}{R_{1,2}}+\frac{N-4}{R_{3,1}}\right]\mathbb{1}\Bigg\}.
\end{aligned} \tag{A.14}$$

For a chain of length N (N odd), the matrix (A.14) is of size $[\frac{N}{2}]\times[\frac{N}{2}]$. It is straightforward to take the matrix elements of this matrix between the first order eigenstates (A.12). We omit the explicit form of this second order expression because it would be almost as long as (A.14).

Appendix B: Proof of the symmetries of the Hamiltonian

This appendix contains a proof of the last line of (5.4.7).

In order to show the third line of (5.4.7) we look at the action of the Hamiltonian (3.1.1) on the states (3.1.11):

$$\begin{aligned} H_N^{(n)} \| i_1 \dots i_N \rangle\rangle_P &= -\left(\sum_{j=1}^{N} \sum_{k=1}^{n-1} \bar{\alpha}_k \omega^{k\, i_j} \right) \| i_1 \dots i_N \rangle\rangle_P \\ &- \lambda \sum_{\{a_1,\dots,a_N\}} \sum_{k=1}^{n-1} \alpha_k V_{k,\{i_1,\dots,i_N\}}^{\{a_1,\dots,a_N\}} e^{iP_{\mathrm{m},Q} f_{k,\{i_1,\dots,a_N\}}^{\{a_1,\dots,a_N\}}} e^{i(P-P_{\mathrm{m},Q}) g_{k,\{i_1,\dots,a_N\}}^{\{a_1,\dots,a_N\}}} \| a_1 \dots a_N \rangle\rangle_P \end{aligned} \tag{B.1}$$

where the $\| a_1 \dots a_N \rangle\rangle_P$ form a suitable basis of the space with momentum P and charge Q. The $f_{k,\{i_1,\dots,a_N\}}^{\{a_1,\dots,a_N\}}$ and $g_{k,\{i_1,\dots,a_N\}}^{\{a_1,\dots,a_N\}}$ are certain integers depending on the choice of basis. The $V_{k,\{i_1,\dots,i_N\}}^{\{a_1,\dots,a_N\}}$ are certain *real* constants. The crucial step in the derivation of the above identity is to show that the basis can be chosen such that

$$f_{k,\{i_1,\dots,a_N\}}^{\{a_1,\dots,a_N\}} = kQ^{-1} \tag{B.2}$$

if $Q^{-1} \in \mathbb{Z}_n$. The existence of a basis $\| a_1 \dots a_N \rangle\rangle_P$ satisfying (B.1) and (B.2) can be seen as follows. Starting from an arbitrary state with charge Q and momentum P, e.g. the state $\| s^Q \rangle\rangle_P$ defined in (4.2.2), one can iteratively *define* the phase factors of the new basis vectors $\| a_1 \dots a_N \rangle\rangle_P$ appearing in (B.1) such that (B.2) holds. It remains to check that this definition is consistent which is equivalent to showing that a basis vector which is already introduced turns up with the proper phase factor in (B.1). Since all states $\| a_1 \dots a_N \rangle\rangle_P$ and $\| b_1 \dots b_N \rangle\rangle_P$ with $0 = \sum_{j=1}^{N} a_j - b_j$ have an equivalent behaviour under the action (B.1) of the Hamiltonian, one can restrict to the states $\| s^Q \rangle\rangle_P$ when checking consistency.

Let us now consider the states $\| s^Q \rangle\rangle_P$ more closely. First we observe that one application of the potential V has contributions also to $\| s^Q \rangle\rangle_P$. The two relevant terms in $V \| s^Q \rangle\rangle_P$ are $\alpha_Q e^{iP} \| s^Q \rangle\rangle_P$ and $\alpha_{n-Q} e^{-iP} \| s^Q \rangle\rangle_P$. These phase factors are compatible with (B.1) and (B.2) because $e^{i2P_{\mathrm{m},Q}}$ is an nth root of unity. Now it remains to check that iterations of (B.2) that do not lead to states $\| s^Q \rangle\rangle_P$ in intermediate steps yield the correct phase factors. It is easy to see that the only non-trivial conditions come from iterations of type

$$\| s^Q \rangle\rangle_P \underset{\alpha_{k_1}}{\mapsto} \| (Q+k_1)(-k_1)0\dots \rangle\rangle_P \underset{\alpha_{k_2}}{\mapsto} \| (Q+k_1+k_2)(-k_1-k_2)0\dots \rangle\rangle_P \dots \underset{\alpha_{k_r}}{\mapsto} \| s^Q \rangle\rangle_P \tag{B.3}$$

without a final shift in the state $\| s^Q \rangle\rangle_P$. The choice (B.2) for Q^{-1} an integer is obviously consistent with eq. (B.1) since $\sum_{s=1}^{r} k_s$ has to be a multiple of n if $\| s^Q \rangle\rangle_P$ is required to reappear without a shift in (B.3). This concludes the proof that one can indeed choose a basis such that (B.2) is valid.

The isomorphism stated in (5.4.7) can now be read off from the following actions of $H_N^{(n)}$ and $(H_N^{(n)})^+$:

$$
\begin{aligned}
H_N^{(n)} \| i_1 \dots i_N \rangle\rangle_{\,P_{\mathrm{m},Q}+P} &= -\left(\sum_{j=1}^{N} \sum_{k=1}^{n-1} \bar{\alpha}_k \omega^{k\, i_j} \right) \| i_1 \dots i_N \rangle\rangle_{\,P_{\mathrm{m},Q}+P} \\
&\quad -\lambda \sum_{\{a_1,\dots,a_N\}} \sum_{k=1}^{n-1} \alpha_k V_{k,\{i_1,\dots,i_N\}}^{\{a_1,\dots,a_N\}} e^{iP_{\mathrm{m},Q} Q^{-1} k} e^{iPg_{k,\{i_1,\dots,a_N\}}^{\{a_1,\dots,a_N\}}} \| a_1 \dots a_N \rangle\rangle_{\,P_{\mathrm{m},Q}+P}\,, \\
(H_N^{(n)})^+ \| i_1 \dots i_N \rangle\rangle_{\,P_{\mathrm{m},Q}-P} &= -\left(\sum_{j=1}^{N} \sum_{k=1}^{n-1} \bar{\alpha}_{n-k} \omega^{-k\, i_j} \right) \| i_1 \dots i_N \rangle\rangle_{\,P_{\mathrm{m},Q}-P} \\
-\lambda \sum_{\{a_1,\dots,a_N\}} \sum_{k=1}^{n-1} \alpha_k V_{k,\{i_1,\dots,i_N\}}^{\{a_1,\dots,a_N\}} & e^{-i2\pi z k} e^{-iP_{\mathrm{m},Q} Q^{-1} k} e^{iPg_{k,\{i_1,\dots,a_N\}}^{\{a_1,\dots,a_N\}}} \| a_1 \dots a_N \rangle\rangle_{\,P_{\mathrm{m},Q}-P}\,.
\end{aligned}
\tag{B.4}
$$

In (B.4) we have used $\bar{\alpha}_k^* = \bar{\alpha}_{n-k}$ and $\alpha_k^* = e^{-2\pi i z k} \alpha_k$. We would like to conclude the proof by noting that for very particular values of the momentum P and the chain length N some of the eigenstates $\| a_1 \dots a_N \rangle\rangle_{\,P}$ in (B.4) might turn out to be identically zero. In this case, the last line of (5.4.7) is strictly true only after inserting projection operators.

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Translations of citations

Aristotle, "The Physics":

In all sciences that are concerned with principles or causes or elements, it is acquaintance with these that constitutes knowledge or understanding. For we conceive ourselves to know about a thing when we are acquainted with its ultimate causes and first principles, and have got down to its elements. Obviously, then, in the study of Nature too, our first object must be to establish principles.

Immanuel Kant, Preface to the second edition of "The Critique of Pure Reason":

Mathematics and physics are the two theoretical sciences which have to determine their objects a priori. The former is purely a priori, the latter is partially so, but is also dependent on other sources of cognition.

Werner Heisenberg:

So far we do not know yet in which language we can talk about events in the atom. We have a mathematical language, i.e. a mathematical scheme, which allows us to compute the stationary states of the atom or the probabilities of a transition from one state to another. But we do not know yet –at least not in general– how this language is connected with the usual language.

Niels Bohr:

On the other hand we encounter difficulties which lie so deep that we do not have any idea of the way of their solution; it is my personal opinion that these difficulties are of such a nature that they hardly allow us to hope that we shall be able, inside the world of the atoms, to carry through a description in space and time of the kind that corresponds to our ordinary images.

H.A. Lorentz:

All this has great beauty and extreme importance, but unfortunately we do not really understand it. We do not understand Planck's hypothesis concerning oscillators nor the exclusion of the nonstationary orbits, and we do not understand, how, after all, according to Bohr's theory, light is produced. There can be no doubt, a mechanics of quanta, a mechanics of discontinuities, has still to be made.