Phase diagram and two-particle structure of the $Z_3$-chiral Potts model

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Abstract: We calculate the low-lying part of the spectrum of the $Z_3$-symmetrical chiral Potts quantum chain in its self-dual and integrable versions, using numerical diagonalisation of the hamiltonian for $N \leq 12$ sites and extrapolation $N \to \infty$. From the sequences of levels crossing we show that the massive phases have oscillatory correlation functions. We calculate the wave vector scaling exponent. In the high-temperature massive phase the pattern of the low-lying levels can be explained assuming the existence of two particles, with $Z_3$-charge $Q = 1$ and $Q = 2$, and their scattering states. In the superintegrable case the $Q = 2$-particle has twice the mass of the $Q = 1$-particle. Exponential convergence in $N$ is observed for the single particle gaps, while power convergence is seen for the scattering levels. In the high temperature limit of the self-dual model the parity violation in the particle dispersion relation is equivalent to the presence of a macroscopic momentum $P_m = \pm \varphi/3$, where $\varphi$ is the chiral angle.
1 Introduction

The $Z_3$-symmetrical chiral clock model ("CC$_3$-model") has been introduced in 1981 in order to describe the transition between commensurate and incommensurate phases of adsorbed gases on crystal surfaces [1, 2, 3]. It is a two-dimensional model defined by the partition function $Z$ and the action $S$:

$$Z = \sum_{\{a\}} \exp(-S)$$
$$S = -\sum_{x,y} \left( g_x \cos[\frac{2\pi}{3}(a_{x+1,y} - a_{x,y})] + g_y \cos[\frac{2\pi}{3}(a_{x,y+1} - a_{x,y}) - \varphi] \right). \quad (1.1)$$

The $Z_3$-spin variables at sites $(x, y)$ take the values $a_{x,y} = 0, 1, 2$. $g_x$ and $g_y$ are the horizontal and vertical couplings, respectively. For non-zero chiral angle $\varphi$ the system is parity-noninvariant in the $y$-direction. For $\varphi = 0$, (1.1) is the usual $Z_3$-clock model.

Various techniques have been used in order to determine the phase diagram of the model: Mean field, Monte-Carlo, renormalization group, partial transfer matrix diagonalization, and hamiltonian limit finite-size calculations [7]-[11]. As yet, no full agreement has been reached between various authors on the details of the phase diagram.

The CC$_3$-model is not self-dual. A self-dual model which should show commensurate-incommensurate phase transitions was proposed and studied by Howes, Kadanoff and Den Nijs in 1983 [12]. Their model is defined by the following quantum chain hamiltonian (or logarithm of the transfer matrix):

$$\mathcal{H} = -\frac{2}{\sqrt{3}} \sum_{j=1}^{N} \left\{ e^{-i\varphi/3} \sigma_j + e^{i\varphi/3} \sigma_j^+ + \lambda \left( e^{-i\phi/3} \Gamma_j \Gamma_{j+1}^+ + e^{+i\phi/3} \Gamma_j^+ \Gamma_{j+1} \right) \right\}, \quad (1.2)$$

where $\sigma_j$ and $\Gamma_j$ are $3 \times 3$-matrices acting at site $j$ (the $Z_3$-analog of the $Z_2$-Pauli matrices $\sigma^z$ and $\sigma^+$):

$$\sigma_j = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}_j, \quad \Gamma_j = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_j \quad (1.3)$$

with $\omega = \exp(2\pi i/3)$. $\mathcal{H}$ contains the three parameters $\lambda$, $\phi$ and $\varphi$. $\lambda$ is the inverse temperature, $\phi$ and $\varphi$ are two chiral angles. For $\phi = \varphi$ the model is self-dual.

For $\phi = 0$ or $\varphi = 0$ the hamiltonian $\mathcal{H}$ follows from the CC$_3$-action (1.1) [12], but for general $\varphi$ and $\phi$ the corresponding two-dimensional lattice model has complex Boltzmann weights, so that there is no straightforward statistical mechanics interpretation. Because of some symmetries of $\mathcal{H}$, it suffices to consider only $0 \leq \phi, \varphi \leq \pi$.

The spectrum of $\mathcal{H}$ decomposes into three charge sectors $Q = 0, 1, 2$ because $\mathcal{H}$ commutes with the $Z_3$ charge operator $\hat{Q} = \prod_{j=1}^{N} \sigma_j$ and we may write the eigenvalues...
of $\hat{Q}$ as $\exp(2\pi i Q/3)$. Although for $\phi \neq 0$, parity is violated, $\mathcal{H}$ is still translational invariant (we use periodic boundary conditions $\Gamma_{N+1} = \Gamma_1$) and the eigenstates will be labeled by the momentum eigenvalues $p$:

$$p = -\left\lfloor \frac{N}{2} \right\rfloor, \ldots, -1, 0, 1, \ldots, \left\lfloor \frac{N}{2} \right\rfloor.$$  

(1.4)

Using perturbation expansions and fermionic techniques, Howes et al. concluded that the phase diagram of the self-dual model ($\varphi = \phi$) contains three phases: an ordered and a disordered phase separated by a $Z_3$-Potts universality class line for low values of $\varphi$, and an incommensurate (IC)-phase for large $\varphi$. However, the most exciting result of their analysis (they used a 10th-order high-temperature expansion) was that for $\varphi = \pi/2$ the lowest gap of $\mathcal{H}$ is a linear function of $\lambda$ (the 2nd to 10th-order coefficients in $\lambda$ were all found to vanish), just as it is the case for the Ising model.

More precisely, let us define the gaps of $\mathcal{H}$ with respect to the lowest $Q=0$, $p=0$-level, which we denote by $E_0(Q=0, p=0)$. Observe that $E_0(Q=0, p=0)$ is not always the ground state of $\mathcal{H}$, since the model has an IC-phase region where in general the ground state carries non-zero momentum $p$.

By $\Delta E_{Q,i}$ we denote the energy difference

$$\Delta E_{Q,i} = E_i(Q, p=0) - E_0(Q=0, p=0)$$  

(1.5)

where $E_i(Q, p=0)$ is the $i$th level ($i = 0, 1, \ldots$) of the charge $Q$, zero-momentum sector. Then the Howes et al. result is

$$\Delta E_{1,0} = 2(1 - \lambda) \quad \text{for}\ \lambda < 1.$$  

(1.6)

In 1984, v.Gehlen and Rittenberg [13] looked into the question, whether also other gaps of the Howes et al. model might be linear in $\lambda$. They found that indeed this is the case. They also constructed a whole series of $Z_n$-symmetrical models which have gaps linear in $\lambda$. These models are defined by the quantum hamiltonians

$$H = -\sum_{j=1}^{N} n^{-1} \sum_{k=1}^{n-1} \left\{ \alpha_k \sigma_j^k + \lambda \alpha_k \Gamma_j^k \Gamma_{j+1}^{-k} \right\}.$$  

(1.7)

Here $\sigma_j$ and $\Gamma_j$ are $n \times n$-matrices acting at site $j$ (the $Z_n$-generalizations of (1.3)) which satisfy

$$\sigma_j \Gamma_{j'} = \Gamma_{j'} \sigma_j \omega^{j-j'}, \quad \sigma_j^n = \Gamma_j^n = 1, \quad \omega = \exp(2\pi i/n).$$  

(1.8)

The $Z_2$-version of (1.7) is the standard Ising quantum chain.

The linearity of gaps is obtained if in (1.7) we choose

$$\alpha_k = \bar{\alpha}_k = 1 - i \cot(\pi k/n).$$  

(1.9)

At the same time eq.(1.9) guarantees [13] that the models (1.7) are integrable in the sense that they satisfy the Dolan-Grady conditions [14], which are equivalent [15] to
the Onsager algebra \[16, 17, 18\]. This kind of integrability is now usually referred to as ”superintegrability” \[19, 20\]. It ensures that if \(\alpha_k, \bar{\alpha}_k\) satisfy eq. (1.9), then the \(\lambda\)-dependence of all eigenvalues \(E(\lambda)\) of \(H\) has the special Ising-like form \[19, 15\]:

\[
E(\lambda) = a + b\lambda + \sum_j 4m_j\sqrt{1 + \lambda^2 + 2\lambda \cos \theta_j}. \tag{1.10}
\]

Here \(a, b\) and \(\theta_j\) are real numbers and the \(m_j\) take the values \(m_j = -s_j, -s_j + 1, \ldots, s_j\) with \(s_j\) a finite integer. For details on formula (1.10) see \[19, 15\].

In 1989 Au-Yang et al. \[21, 22\] derived the hamiltonian (1.7) from a two-dimensional lattice model built out of \(Z_n\)-symmetrical (but not generally positive) Boltzmann weights. These satisfy a new kind of Yang-Baxter equations with the spectral parameters defined on a Riemann surface of high genus. In a series of papers, the authors of \[21-26\] have been able, using in addition a functional equation \[27\], to calculate the complete spectrum of the \(Z_3\)-hamiltonian (1.2) in the superintegrable case \(\phi = \varphi = \pi/2\).

From the Yang-Baxter equations it follows that (1.7) is also integrable if the \(\alpha_k\) and \(\bar{\alpha}_k\) satisfy the relations

\[
\alpha_k = e^{i(2k/n-1)\varphi} / \sin(\pi k/n), \quad \bar{\alpha}_k = e^{i(2k/n-1)\phi} / \sin(\pi k/n), \tag{1.11}
\]

\[
\cos \varphi = \lambda \cos \phi \tag{1.12}
\]

Except for the superintegrable case, which is contained in (1.12) for \(\phi = \varphi = \pi/2\), these equations force \(H\) to be non-self-dual. Calculating the spectrum for the integrable, but not superintegrable case (1.11), (1.12) is a very difficult task. Nevertheless some initial steps have been done in attacking this problem \[28\].

In this talk, we shall give some new results on the \(Z_3\)-model (1.2). We shall not rely on exact solutions and calculate low-lying energy levels of \(H\) by numerical diagonalization (using the Lanczos algorithm) of the chain hamiltonian for up to \(N = 12\) sites. The motivation for such a work is two-fold:

1) For the superintegrable case, where exact results are available, the numerical evaluation of the exact formulae is not easy, and straightforward numerical diagonalization sometimes gives more transparent results on the behaviour of whole sets of levels. This may lead to the discovery of regularities which otherwise could be overlooked. Indeed, a good fraction of the progress in finding the special properties of (1.7) has been made possible by the extensive finite-size studies performed by the authors of \[13, 29\].

2) Of course, the main merit of the finite-size method is, that it is not restricted to the superintegrable case and so one can study how the special superintegrable spectrum emerges from the \(\varphi\)-dependence of the general spectrum.

In the next Section we shall show that the massive phases are oscillatory, Sec. 3 gives a calculation of the corresponding wave-vector scaling critical index, which sheds new light on the scaling asymmetry noticed in \[29, 24\]. Sec. 4 then interprets the low-lying spectrum of the massive phases in terms of ”elementary” particles and their composite states. Sec. 5 summarizes our results.
2 Oscillatory behaviour of the massive phases

Due to its complex coefficients, the hamiltonian (1.2) allows ground state level crossings (the Perron-Frobenius theorem does not apply). The different phases can be easily distinguished by the $Z_3$-charge sectors and momenta of the lowest energy levels of $\mathcal{H}$. In Fig. 1 for fixed number of sites $N = 10$ we draw a map of the $\lambda/\phi$- plane (in order not to get lost on three-dimensional figures, in the following we shall consider the self-dual case $\phi = \varphi$ if not explicitly stated otherwise). We label regions in this plane by the sectors of the two lowest levels, e.g. $0_1/2_3$ means that the ground state is in the $Q=0, p=1$-sector and the first excited state has $Q=2, p=3$. In most cases the lines mark alternately cross-overs in the ground state and in the first excited state.

Fig. 1: Map of the lines where cross-overs in the two lowest levels of the hamiltonian (1.2) (self-dual version $\varphi = \phi$) for $N = 10$ sites occur. The meaning of the labelling of the regions between the cross-overs is explained in the text.
Fig. 2: Schematic phase diagram of the self-dual version of the $Z_3$-chiral Potts model defined by the hamiltonian eq. (1.2).

Inspection of Fig. 1 shows that there are at least 3 different phases (Fig. 2 gives a general schematic view of the phase diagram):

- Low-temperature phase (I) at $\lambda > 1$ and small $\phi$: Here the three lowest states are from three different charge sectors and belong to the zero momentum sector. As $\lambda$ increases at fixed $\phi$, the three levels form a kind of braid and alternate in forming the ground state. We mention that the gaps between the braiding levels decrease exponentially both with $N$ and $\lambda$, as it is expected for the low-temperature phase where the ground state is threefold degenerate in the thermodynamic limit $N \to \infty$ (the next levels follow at the distance of $\Delta E \approx 3(\lambda - 1)$ as has been shown by Baxter [24]).

In their low-$\phi$-branches the cross-over lines follow a simple pattern for $\lambda \to \infty$: all these lines tend to fixed values of $\phi$ according to the rule [31] (which we verified numerically):
$0_0/1_0$ (crossing in the ground state) $\Rightarrow \varphi = \pi/N$

$0_0/2_0$ (crossing in the 1st excited state) $\Rightarrow \varphi = 2\pi/N$

$1_0/2_0$ (ground state) $\Rightarrow \varphi = 3\pi/N$

$1_0/0_0$ (1st excited state) $\Rightarrow \varphi = 4\pi/N$

$2_0/0_0$ (ground state) $\Rightarrow \varphi = 5\pi/N$

$2_0/1_0$ (1st excited state) $\Rightarrow \varphi = 6\pi/N$ etc.

These rules are teaching us that for $N \to \infty$ there will be an infinite supply of cross-over lines, which finally will fill the whole region $\lambda > 1$ down to $\varphi = 0 + \epsilon$.

We have also verified that for free b.c. (and also for the integrable version of the model) the same asymptotic behaviour of the cross-over lines appears. So these cross-overs are not just artefacts of the boundary condition. We conclude that this phase is an oscillatory massive phase. In the next Section we shall give evidence that for increasing $N$ the cross-over lines converge to the line $\lambda = 1$ and give the calculation of the wave vector critical index.

• High-temperature phase (II). Dual to phase (I) this appears at $\lambda < 1$ and small $\varphi$. Here the ground state always belongs to the sector $Q=0, p=0$ so that there are no ground state level crossings. However, there is a regular pattern of cross-overs in the first excited state, which is always in $Q=1$, but with increasing $N$ and $\varphi$ switches to higher momenta. Perturbation theory in $\lambda$ teaches us that at $\lambda = 0$ the first excited state moves from momentum $p_0$ to $p_1$ at the chiral angle

$$\varphi = \frac{3\pi}{N}(p_0 + p_1).$$

(2.1)

Again, this rule ensures that for $N \to \infty$ there is an infinite supply of cross-over lines, this time in the first excited level. This gives rise to a modulation of $\Delta p \neq 0$-pair correlation functions (the $\Delta p = 0$-pair correlations are non-oscillatory).

• Massless incommensurate phases (III, IV): In the middle upper part of the phase diagram there are plenty of ground- and first-excited state level crossings. Both the charge sectors and the momenta are changing simultaneously. With increasing $N$ the pattern of cross-over lines becomes more dense. The loss of translational invariance of the ground state together with a $\lambda$-dependent variation of the ground state momentum is sign of the presence of an incommensurate (IC)-phase.

Here the information from the exact solution of Albertini et al. [19] on the line $\varphi = \pi/2$ provides more detailed information than we are able to obtain from our chains of $N \leq 12$ sites: In [19] it is shown that on the superintegrable line the ground state looses translational invariance in the interval $0.901293 \leq \lambda \leq 1/0.901293$. In [30] in addition it is shown that actually for $\lambda < 1$ and $\lambda > 1$ there are two different IC-phases which do not join smoothly at $\lambda = 1$. 

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The appearance of \( p \neq 0 \) in the first excited state in the high-temperature region is an indication that eventually the ground state may acquire momentum too, but \( N \leq 12 \) sites are not enough to prove that this happens already on the line \( \varphi = \pi/2 \).

Interesting information is obtained from our calculations on the different behaviour of the self-dual (\( \varphi = \phi \)) and integrable (\( \cos \phi = \lambda \cos \varphi \)) hamiltonians for \( \lambda > 1 \) and \( \varphi \rightarrow \pi \): In the integrable case we find that the ground state cross-over lines for \( \varphi \rightarrow \pi \) concentrate below \( \lambda \approx 1.6 \) and no cross-overs are left at \( \varphi = \pi \) above this value of \( \lambda \). This is in contrast to the self-dual case, where the cross-over lines for \( \varphi \rightarrow \pi \) spread out to \( \lambda = \infty \). In agreement with the phase diagram drawn by Roan and McCoy \([28]\), we conclude that in the integrable case, phase (I) extends up to \( \varphi = \pi \) and \( \lambda \approx 1.6 \).

For the self-dual case we are able to determine the boundary between phases (I) and (IV) with good precision, because the lowest gaps in region (I) are exponentially small as mentioned above, whereas the gaps in the IC-region are generally of order unity. In Tables 1 and 2 we give an idea of the precision with which the phase boundary to the IC-phases can be determined by our finite-size extrapolation \([31]\).

| \( N \) | \( \lambda = 0.1 \) | 0.25 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 |
|-------|----------------|-----|-----|-----|-----|-----|-----|
| 9     | 170.860        | 157.553 | 135.605 | 127.301 | 119.986 | 114.519 | 112.333 |
| 10    | 171.112        | 158.085 | 135.767 | 126.779 | 118.457 | 111.796 | 108.522 |
| 11    | 171.358        | 158.649 | 136.252 | 126.751 | 117.556 | 109.763 | 105.366 |
| 12    | 171.589        | 159.208 | 136.927 | 127.060 | 117.121 | 108.263 | 102.728 |
| \( \infty \) | 170.43(4) | 157.1(1) | 135.7(2) | 126.3(3) | 115.1(1) | 103.7(1) | 87.6(7) |

Table 1. : Determination of the phase boundary between the high-temperature phase II and the IC-phase IV from the first crossing of the levels \( 0_0 \) and \( 1_1 \). For brevity, we quote only the values for \( N = 9, \ldots, 12 \). However, in estimating the limiting values denoted ”\( \infty \)”, data for all sites \( N = 3, \ldots, 12 \) have been used. The estimated errors of the last given digit are quoted in brackets.

| \( N \) | \( \lambda = 1.1 \) | 1.2 | 1.4 | 1.6 | 1.8 | 2.2 | 2.6 | 3.0 |
|-------|----------------|-----|-----|-----|-----|-----|-----|-----|
| 9     | 120.007        | 124.409 | 132.599 | 143.899 | 150.729 | 155.270 | 158.526 |
| 10    | 116.541        | 121.733 | 131.092 | 143.357 | 150.491 | 155.149 | 158.457 |
| 11    | 113.703        | 119.695 | 130.146 | 143.192 | 150.521 | 155.232 | 158.553 |
| 12    | 111.355        | 118.152 | 129.613 | 143.278 | 150.718 | 155.438 | 158.746 |
| \( \infty \) | 99.(1) | 113.2(1) | 127.8(2) | 144.(1) | 151.2(2) | 156.(2) | 159.(1) |

Table 2. : Determination of the phase boundary between the low-temperature phase I and the IC-phase III from the first crossing of the levels \( 1_0 \) and \( 2_2 \).
Whether these transition lines have the properties of a Pokrovski-Talapov type transition \[32\] is an interesting open question, because here two modulated phases have to coexist at the phase boundary line.

3 Determination of the wave vector scaling exponent

In this section we shall take a closer look at the \(N\)-dependence of the level crossings in the low-temperature region \(\lambda > 1\). In Table 3 we give the cross-over positions in \(\lambda\) for the superintegrable case which appear for \(N\) up to 12 sites.

This Table shows that the cross-over lines converge towards \(\lambda = 1\) and not towards the I/III-phase boundary \(\lambda = 1.109518\). So the low-lying \(p = 0\)-levels and their cross-overs do not care about the point where the IC-phase sets in. Between \(\lambda = 0.901293\) and \(\lambda = 1/0.901293\) just the \(p = 0\)-levels are no longer the lowest levels. This is analogous to the formula (1.6) for the \(p = 0\)-gap valid for \(\lambda < 1\) which also takes no notice of the point \(\lambda = 0.901293\).

| \(N\) | \(Q=0/1/2\) | 1/0/2 | 1/2/0 | 2/1/0 | 2/0/1 |
|------|-------------|-------|-------|-------|-------|
| 3    | 1.8789156   |       |       |       |       |
| 4    | 1.3645610   |       |       |       |       |
| 5    | 1.2201036   | 3.3430364 |       |       |       |
| 6    | 1.1368767   | 2.0826986 |       |       |       |
| 7    | 1.0978185   | 1.6742233 | 4.8041526 |       |       |
| 8    | 1.0738838   | 1.4761904 | 2.8030552 |       |       |
| 9    | 1.0580721   | 1.3610533 | 2.1459063 | 6.2689052 |       |
| 10   | 1.0470391   | 1.2866459 | 1.8229750 | 3.5290793 |       |
| 11   | 1.0390113   | 1.2350807 | 1.6327694 | 2.6244231 |       |
| 12   | 1.0329732   | 1.1975179 | 1.5083542 | 2.1772063 | 4.255 |
| \(\infty\) | 0.9997(5) | 0.999(1) | 0.990(6) | 0.93(5) |       |

Table 3. Positions in \(\lambda\) of the \(p = 0\)-sector lowest level crossings on the superintegrable line \(\varphi = 90^\circ\) for periodic b.c. In the top line the order of the levels with different charges \(Q\) in the \(\lambda\)-interval between the cross-overs is given. So the first column of \(\lambda\)-values gives the position of the \(0_0/1_0\)-cross-over, the second column the \(0_0/2_0\)-cross-over in the first excited state, etc.

Critical exponents of the translationally invariant part of the spectrum at \(\lambda = 1\) have been discussed in \[29, 24\]. These authors find that scaling is asymmetrical around \(\lambda = 1\) and derived the specific heat exponent to be \(\alpha = 1 - 2/n\) for the \(Z_n\)-superintegrable models. From (1.6) it is immediate that the magnetic critical index is \(\nu = 1\). The spacial correlation exponent \(\nu_s\) has been calculated by Albertini et al. \[29\] from the \(\lambda\)- and \(N\)-dependence of the \(Q = 0, p = 0\)-"ground"-state alone to be \(\nu_s = 2/n\). Baxter \[24\] finds from the exact solution of the superintegrable model the
same value $2/n$ for the interfacial tension exponent which describes the exponential approach in $N$ to degeneracy of the $p = 0$-lowest levels in the low-temperature phase near $\lambda = 1$.

We want to show that in the $Z_3$-case (1.2) one obtains $\nu_s = 2 \over 3$ for the wave vector exponent at $\lambda = 1$. We are not restricted by our method to the superintegrable point and find that $\nu_s$ varies little or not at all for a wide range of the chiral angle $\varphi$. All our results are consistent with the hypothesis that it is the inverse wave vector which sets the dominant spacial scale length of the $p = 0$ sector of the spectrum around $\lambda = 1$.

The finite-size scaling rules for quantum chains with oscillating phases have been formulated in [33]. Let us define $\nu_s$ as the power of divergence of the inverse wave vector as $\lambda \to \lambda_c$:

$$1/K \sim (\lambda - \lambda_c)^{-\nu_s}. \quad (3.1)$$

In the region dominated by the length scale $1/K$ we use the scaling variable

$$z = N^{1/\nu_s}(\lambda - \lambda_c) \quad (3.2)$$

From Table 3 we deduce that $\lambda_c = 1$. In the scaling regime we can express the cross-over positions $\lambda_k(N)$ ($k = 1, 2, \ldots$) in terms of values $z_k$ of the scaling variable. Calling $\Lambda_{k,k'}(N)$ the distance between two level crossing points (e.g. at fixed $\varphi$) we can write

$$\Lambda_{k,k'}(N) \equiv \lambda_k(N) - \lambda_{k'}(N) = (z_k - z_{k'})N^{-1/\nu_s}. \quad (3.3)$$

Using eq.(3.3) for $N$ and $N - 1$ sites, we get $N$th approximants for $\nu_s$:

$$\nu_s(N, k, k') = \frac{\ln(N/(N - 1))}{\ln \frac{\Lambda_{k,k'}(N-1)}{\Lambda_{k,k'}(N)}}. \quad (3.4)$$

If our assumptions are consistent, the large $N$-limit of these approximants has to give the same value $\nu_s$ for every choice of pairs $k, k'$:

$$\nu_s = \lim_{N \to \infty} \nu_s(N, k, k'). \quad (3.5)$$

One may also refer the distances to $\lambda_c = 1$ and use $\Lambda_{k,0}(N) = \lambda_k(N) - \lambda_c$ in (3.4), corresponding to $z_0 = 0$ in (3.3).

In Table 4 we give numerical results from three different choices of $\Lambda_{k,k'}$. Observe that from $\varphi = 120^\circ$ down to $\varphi = 60^\circ$ we find no appreciable variation of $\nu_s$ with $\varphi$. In particular, there is no indication of a rise towards the $\varphi = 0$-Potts value $\nu_s = 5 \over 6$. Unfortunately, for small $\varphi$ the cross-over lines move to large $\lambda$ for our small $N$ available, so that the convergence of the $\nu_s(N, k, k')$ becomes poor e.g. for $\varphi = 30^\circ$.

From the level crossing points and the slopes of the gaps at these points, we can also obtain information on the specific heat exponent $\alpha$ and the magnetic gap exponent $\nu$ [33]. The specific heat $C_v$ and its exponent $\alpha$ are defined by

$$C_v(\lambda) = -\frac{1}{N} \frac{d^2 E_0}{d\lambda^2} \sim |\lambda_c - \lambda|^{-\alpha}. \quad (3.6)$$

In the region with ground-state cross-overs, its finite-size approximants $C_v(\lambda, N)$ are
The weight factors of the $\delta$-terms are given by the $\lambda$-derivatives of the magnetic gaps at the ground state cross-over positions:

$$C_k(N) = \frac{1}{N} \left| \frac{d(E_{Q_i} - E_{Q_j})}{d\lambda} \right|_{\lambda_k(N)}. \quad (3.8)$$

The relevant charge sectors $Q_i, Q_j$ rotate as $\lambda$ increases, see Table 3.

In the scaling regime we express $C_v(\lambda, N)$ in terms of the specific heat scaling function $C(z)$

$$C_v(\lambda, N) = N^{\alpha/\nu_s} C(z) = N^{\alpha/\nu_s} \sum \bar{C}_k \delta(z - z_k), \quad (3.9)$$

so that

$$C_k(N) = \bar{C}_k N^{(\alpha-1)/\nu_s}. \quad (3.10)$$

From (3.10) we get approximants $\alpha(N, k)$ for $\alpha$:

$$\alpha(N, k) - 1 = \nu_s(N, k) \ln \left( \frac{C_k(N - 1)}{C_k(N)} \right) / \ln \left( \frac{N - 1}{N} \right) \quad (3.11)$$

Formula (3.11) gives a practicable method for calculating $\alpha$ from the $\nu_s(N, k)$ and the $(\Delta Q \neq 0)$-magnetic gap slopes (3.8).
The fact that the specific heat contributions from the ground-state crossings are proportional to magnetic gap slopes gives rise to the generalized hyperscaling relation \[33\]-\[37\]:
\[
\alpha + \nu_s + \nu = 2, \tag{3.12}
\]
which is easily seen to be valid even for the finite-$N$-approximants to $\alpha$, $\nu_s$ and $\nu$ \[33\].

For detailed tables of the relevant sequences of approximants, we refer the reader to \[31\]. Here we just mention that we find $\nu = 1$ within a few percent error for all $60^\circ \leq \varphi \leq 120^\circ$. So for these values of $\varphi$ eq.\((3.12)\) reads $\frac{1}{3} + 1 + \frac{2}{3} = 2$. For the Potts case $\varphi = 0^\circ$ we know that it must read $\frac{1}{3} + \frac{5}{6} + \frac{5}{6} = 2$, but we are not able to tell at which $\varphi$ the first equation goes over to the second one.

4 Particle interpretation of the low-lying spectrum

In this section we attempt to describe the low-lying part of the spectrum of $\mathcal{H}$ of eq.\((1.2)\) in terms of elementary excitations. For the superintegrable case such a discussion has been given e.g. in \[38, 26\], but it is instructive to consider the dependence on the chiral angle too. We shall treat the self-dual case $\varphi = \phi$ if not stated otherwise.

Let us start with the information we have for $\varphi = 0$. This is the standard $\mathbb{Z}_3$-Potts model which has a second order phase transition at $\lambda = 1$ decibed by a $c = \frac{4}{3}$-conformal field theory \[39, 40\]. Zamolodchikov has shown \[41\] that the high-temperature scaling regime around $\lambda = 1$ is described by the thermal perturbation of the $c = \frac{4}{3}$- conformal theory, which, as he showed, is still integrable. The $S$-matrix of this massive theory factorizes and contains just a single pair of particles with $\mathbb{Z}_3$-charges $Q=1$ and $Q=2$. Because of the additional $S_3$-symmetry present at $\varphi = 0$ the $Q=1$ and $Q=2$-sectors are degenerate and consequently both particles have the same mass, forming a particle-antiparticle pair. The higher levels of the high-temperature scaling Potts-model are multiparticle scattering states of which even the phase shifts are known.

In order to find out whether the spectrum for $\varphi \neq 0$ is continuously obtained from the Potts spectrum, we first take a look at a high-temperature expansion of the $p = 0$-states. In the interval $-\frac{\pi}{2} < \varphi < \pi$ we find for the lowest $Q = 1$, $p = 0$-gap up to order $\lambda^2$:

\[
\Delta E_{1,0}(\varphi, \lambda) = 4 \sin \frac{\pi - \varphi}{3} - \frac{4\lambda}{\sqrt{3}} \cos \frac{\varphi}{3} - \frac{2\lambda^2}{\sqrt{3}} \sin \frac{1}{3}(\pi - 2\varphi) f(\varphi) + \ldots \tag{4.1}
\]

Here $f(\varphi)$ is a smoothly varying function of $\varphi$, which satisfies

\[
f(-\frac{\pi}{2}) = 2/\sqrt{3}; \quad f(0) = 1; \quad f(\frac{\pi}{2}) = \sqrt{3}/2; \quad \lim_{\varphi \to \pi} f(\varphi)/\sin \frac{1}{3}(\pi - \varphi) = 2\sqrt{3}. \tag{4.2}
\]

Applying a $CP$-transformation, the same formula can be used for the $Q=2$, $p = 0$-gap if $|\varphi| < \frac{\pi}{2}$:

\[
\Delta E_{2,0}(\varphi, \lambda) = \Delta E_{1,0}(-\varphi, \lambda). \tag{4.3}
\]
For small values of $\lambda$, for which these formulae are useful, the level $E_0(Q=1, p=0)$ is isolated in the spectrum of the $Q=1$-charge sector if $0 \leq \varphi < \pi$. Similarly, the level $E_0(Q=2, p=0)$ is isolated in the spectrum of the charge sector $Q=2$ for $0 \leq \varphi < \frac{\pi}{2}$. So we tentatively call these two levels ”single particle levels” and assign the masses

$$m_1 \equiv \Delta E_{1,0}; \quad m_2 \equiv \Delta E_{2,0}. \quad (4.4)$$

For $\varphi \rightarrow 0$ both particles become degenerate, in agreement with our discussion of the Potts case.

Now let us take a look at formulae (4.1) (4.3) for $\varphi \rightarrow \frac{\pi}{2}$. Disregarding first the $\lambda^2$-term, with $\varphi$ increasing, $m_2$ increases faster than $m_1$ decreases. For $\varphi = \frac{\pi}{2}$ (the superintegrable case) we seem to get

$$m_1 = 2 - 2\lambda + O(\lambda^2); \quad m_2 = 4 - 2\lambda + O(\lambda^2). \quad (4.5)$$

While this formula is allright for $m_1$ (we even know that all higher order terms in $\lambda$ vanish as $\varphi \rightarrow \frac{\pi}{2}$) it is not correct for $m_2$, since for $m_2$ the coefficient of $\lambda^2$ diverges as $\varphi \rightarrow \frac{\pi}{2}$. Physically this divergence is not surprising because as $\varphi \rightarrow \frac{\pi}{2}$ particle $m_2$ moves towards the threshold of the two-$m_1$-particle scattering states which are in the same $Q=2$-sector, since the $Z_3$ charges of the particles are additive $\text{mod} \ 3$.

Calculating numerically $m_1$ and $m_2$ for many points of the region $0 \leq \varphi < \frac{\pi}{2}$, $0 \leq \lambda < 1$ we find that there is a smooth change of the ratio $m_2/m_1$ from its Potts-value $m_2/m_1 = 1$ to $m_2/m_1 \rightarrow 2$ as $\varphi$ approaches $\pi/2$ from below.

Since we can easily calculate numerically the about eight lowest $p = 0$ levels of each charge sector for all $0 \leq \varphi \leq \pi$, we now check whether the pattern of higher levels fits to the proposed particle interpretation. In Figs. 3 and 4 we show the expected patterns of levels and thresholds, which should be qualitatively different for $\varphi < \frac{\pi}{2}$ and $\varphi \geq \pi$ if in the latter case $m_2$ becomes larger than $2m_1$.

- **Sector $Q = 0$:** As long as $m_2 < 2m_1$ ($\varphi < \frac{\pi}{2}$), the first threshold is due to the scattering of two different particles $m_1$ and $m_2$, followed at $\Delta E = 3m_1$ by the $3$-$m_1$-particle scattering states (here again we refer the energy gaps to the $Q = 0$, $p = 0$-ground state). This two-particle threshold moves into the $3m_1$-continuum at the superintegrable line if there we have $m_2 = 2m_1$. In Table 5 we give the finite-$N$ energy gaps accessible to our numerical diagonalization of $\mathcal{H}$ for the superintegrable case and $\lambda = 0.5$. We choose this value of $\lambda$ because then from (1.6) we have $m_1 = 1$ and a normalization of the data is unnecessary. The superintegrable case is particularly interesting, because it makes it necessary to disentangle physically different but degenerate levels.

Not surprisingly after this general discussion, in our numerical calculation, the lowest bunch of levels appears at $\Delta E = 3m_1$. Now, in order to find out, which of these levels are $m_1 + m_2$-states and which are the $m_1 + m_1 + m_1$-states, we look into their finite-size behaviour. For a single particle level we expect exponential convergence for $N \rightarrow \infty$:

$$\Delta E(N) - \Delta E(\infty) = \exp(-N/\xi) + \ldots \quad (4.6)$$

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where $\xi$ is a correlation length. In contrast, for multiparticle scattering states we expect power convergence [42, 43]:

$$\Delta E(N) - \Delta E(\infty) \sim N^{-y} + \ldots$$

(4.7)

We calculate approximants $y_n$ to $y$ using neighbouring values of $N$:

$$y_N = \ln \left( \frac{\Delta E(N) - \Delta E(\infty)}{\Delta E(N-1) - \Delta E(\infty)} \right) / \ln \left( \frac{N}{N-1} \right).$$

(4.8)

Table 6 shows some $y_n$ calculated from the $N$-dependence of the energy levels in Tab. 5. We see that the limiting values of $y$ come out clearly to be very close either to $y = 2$ or $y = 3$ and allow us to decide which of the levels are $m_1 + m_2$-states and which are $m_1 + m_1 + m_1$.

• Sector $Q = 1$: Here we see exponential convergence for the isolated level $m_1$, and with good precision we see at $\Delta E = 4$ the bunch of the next higher levels. There are levels converging with $y = 2$ and others converging with $y = 3$. The obvious interpretation is in terms of $m_2 + m_2$-two-particle states and of $m_1 + m_1 + m_2$-three particle states. We have checked that moving towards smaller values of $\varphi$ these levels split in the expected way: for $m_2 < 2m_1$ the levels interpreted as "two-particle" go lower than the assumed three-particle states.

• Sector $Q = 2$: For e.g. $\varphi = 45^\circ$ there is the clear exponential convergence of the isolated $m_2$-level. However, the interesting and crucial test comes now in the superintegrable case: Among the several levels at $\Delta E = 2$ (we still consider $\lambda = 0.5$) which show power convergence, can we distinguish one level which shows exponential behaviour? Already without calculating the sequences $y_n$ we see that the level in the first row of the bottom part of Table 5 sticks out by its very fast convergence. This is substantiated in Table 6 where we see the corresponding sequence of the $y_n$ growing very fast. So we have evidence that the particle $m_2$ survives up to $\varphi = \frac{\pi}{2}$. We have tried to follow $m_2$ into the continuum for $\varphi > \frac{\pi}{2}$. For $\varphi = 105^\circ$ and $\lambda = 0.15$ we have succeeded in distinguishing one level which converges faster than a low power $y = 2$ or $y = 3$.

We have also performed calculations for $\varphi = 45^\circ$, $105^\circ$, both for the self-dual and for the integrable model. In all these cases we find a pattern of the ca.6 lowest levels of each charge sector as sketched in Figs. 3 and 4.

By analogy, we expect that the superintegrable $Z_n$-models have low-lying excitations corresponding to $n-1$ particle species, one in each $Q \neq 0$-sector with mass $m_Q = Qm_1$.

Fig. 3: (following page) General structure of the low-lying spectrum. Left hand side of the picture: Structure of the spectrum in the different charge sectors if the chiral angle $\varphi$ has a value below $\varphi = \frac{\pi}{2}$. Right hand side: for $\varphi$ above the superintegrable value.
(space for Fig. 3)
### Table 5: The lowest energy gaps $\Delta E_{Q,i}$, as defined in eq.(1.5), for the $Z_3$-Hamiltonian eq.(1.2), for the superintegrable case $\phi = \varphi = \pi/2$, and $\lambda = 0.50$. Upper Table: sector $Q = 0$, middle table: sector $Q = 1$ and bottom table: sector $Q = 2$. The numbers given in brackets indicate the estimated error in the last written digit.

| $N$ | $i = 1$ | 2   | 3   | 4   | 5   | 6   |
|-----|---------|-----|-----|-----|-----|-----|
| 6   | 3.2402540 | 5.4035327 | 4.7691472 | 6.4717590 | 6.2844859 |     |
| 7   | 3.1598983 | 4.8359585 | 4.4520381 | 5.9303676 | 5.9032240 | 7.0487030 |
| 8   | 3.1115649 | 4.4240923 | 4.2075367 | 5.4868664 | 5.5496714 | 6.3987521 |
| 9   | 3.0808417 | 4.1213280 | 4.0168334 | 5.1252880 | 5.2384091 | 5.8572524 |
| 10  | 3.0604137 | 3.8954662 | 3.8861605 | 4.8297326 | 4.9700825 | 5.4121174 |
| 11  | 3.0463166 | 3.7244809 | 3.7455652 | 4.5867795 | 4.7406004 | 5.0471104 |
| 12  | 3.0362806 | 3.5932058 | 3.6478379 | 4.3856960 | 4.5447640 | 4.7471645 |
| $\infty$ | 2.9998(3) | 2.986(7) | 3.01(1) | 3.02(8) | 3.05(6) | 2.9(1) |
| $y$ | 3.0(1) | 2.9(2) | 2.0(1) | 2.1(1) | 1.9(1) | 2.8(6) |

| $N$ | $i = 0$ | 1   | 2   | 3   | 4   |
|-----|---------|-----|-----|-----|-----|
| 6   | 0.9963767 | 4.7353052 | 6.1998192 | 7.2942778 | 6.5428730 |
| 7   | 0.9984874 | 4.5173085 | 5.7905491 | 6.6049711 | 6.1612566 |
| 8   | 0.9994289 | 4.3760023 | 5.4775432 | 6.0785242 | 5.8456347 |
| 9   | 0.9998044 | 4.2809972 | 5.2349161 | 5.6757753 | 5.5870148 |
| 10  | 0.9999405 | 4.2150750 | 5.0442562 | 5.3652765 | 5.3749672 |
| 11  | 0.9999851 | 4.1680556 | 4.8924532 | 5.1235743 | 5.2002368 |
| 12  | 0.9999978 | 4.1336962 | 4.7700872 | 4.9335093 | 5.0552644 |
| $\infty$ | 1.0000000 | 3.99(2) | 4.00(1) | 4.01(5) | 4.01(3) |
| $y$ | expon. | 3.0(2) | 2.0(1) | 2.9(2) | 1.9(1) |

| $N$ | $i = 0$ | 1   | 2   | 3   | 4   |
|-----|---------|-----|-----|-----|-----|
| 6   | 2.0002000 | 2.9975868 | 4.8074676 | 5.9788475 | 6.5436728 |
| 7   | 1.9995726 | 2.7901373 | 4.3798245 | 5.6634147 | 6.1294869 |
| 8   | 1.9996761 | 2.6389905 | 4.0256344 | 5.3106885 | 5.8468390 |
| 9   | 1.9998304 | 2.5261089 | 3.7351818 | 4.9697753 | 5.8323103 | 5.6487379 |
| 10  | 1.9999247 | 2.4399607 | 3.4970152 | 4.6583108 | 5.5766919 | 5.5065400 |
| 11  | 1.9999701 | 2.3729391 | 3.3008958 | 4.3808694 | 5.3110577 | 5.4022604 |
| 12  | 1.9999893 | 2.3198948 | 3.1384071 | 4.1365977 | 5.0527923 | 5.3242970 |
| $\infty$ | 2.0001(1) | 2.002(7) | 2.00(5) | 2.0(1) | 2.6(5) | 4.99(1) |
| $y$ | expon. | 2.0(1) | 1.9(1) | 1.9(2) | 2.6(5) | 2.9(2) |
Table 6: Exponents $y_N$ of the convergence $N \to \infty$ as defined in eq.(4.8), for the superintegrable case and $\lambda = 0.50$ for the lower levels given in Table 5. "expon." in the bottom row means that the increasing sequence of the $y_N$ in the column above indicates exponential convergence.

Having been successful with the two-particle interpretation of the low-lying spectrum, we finally consider the energy-momentum relation of these particles. Since parity is generally not a good quantum number of our model, the dispersion relation is not expected to be symmetrical between positive and negative momenta. In [19] such unsymmetrical dispersion curves have been given for the superintegrable case. We have studied the $\varphi$-dependence of this asymmetry. Of course, for $\varphi \to 0$ the asymmetry must vanish because for $\varphi = \phi = 0$ the hamiltonian $H$ is parity invariant. The high-temperature expansion gives us some information about the increase of the asymmetry with $\varphi$ (we consider again the self-dual case):

For calculating the limit $N \to \infty$ using lattice momenta $p$ as in eq.(1.4), we introduce the macroscopic momentum $P$ defined by

$$P = \frac{2\pi}{N} p \quad (-\pi \geq P \geq \pi) \quad (4.9)$$

Then, in generalisation of (4.1), (4.3) we find up to order $\lambda$:

$$\Delta E_{1,0}(\lambda, P) = 4 \sin \frac{\pi - \varphi}{3} - \frac{4\lambda}{\sqrt{3}} \cos(P - \frac{1}{3}\varphi) + \ldots \quad (0 \leq \varphi < \pi) \quad (4.10)$$

and

$$\Delta E_{2,0}(\lambda, P) = 4 \sin \frac{\pi + \varphi}{3} - \frac{4\lambda}{\sqrt{3}} \cos(P + \frac{1}{3}\varphi) + \ldots \quad (0 \leq \varphi < \pi/2). \quad (4.11)$$

This shows that for small $\lambda$, the asymmetry of the energy-momentum relation with respect to $P \to -P$ is due only to the presence of a macroscopic momentum $P_m = \pm \varphi/3$ (observe that this is the same momentum which appears in eq.(2.1) for $\varphi = \frac{\pi}{2}$). We have checked numerically that for $\lambda \leq 0.1$ these formulae are an excellent description of the data. Only for large values of $\lambda$ the situation is getting complicated.
Of course, since we considered just a few low-lying levels, we are not able to make statements about higher levels. In ref. [26] it has been shown that in the superintegrable case the model contains levels which cannot be interpreted as quasiparticles in the sense that their energies and momenta receive unrelated additive contributions.

5 Conclusions

In this talk we reported results of a numerical investigation of the low-lying spectrum of the $Z_3$-chiral Potts hamiltonian (1.2) for $N = 2, \ldots, 12$ sites. We get an overview about the dependence of ca. 18 levels on the chiral angle and the inverse temperature. This fits to the interpretation of the high-temperature low-lying spectrum in terms of two basic particles with $Z_3$-charges $Q = 1$ and $Q = 2$ and their scattering states. The superintegrable case is distinguished by the special $1 : 2$-mass ratio of the particles. Even when moving slightly into the continuum formed by two $Q = 1$-particles, the heavy $Q = 2$-particle can be distinguished by its exponential finite-size behaviour. Two- and three-particle scattering states can be distinguished by their different finite-size power behaviour. High-temperature perturbation theory gives a simple expression for the effect of parity violation on the energy-momentum relation of the particles.

Particular attention has been devoted to the study of ground-state level crossings in the low-temperature regime. We found that the massive phases have oscillatory correlation functions and calculated the wave-vector critical exponent from the low-temperature phase. It turns out that for translation invariant features of the model in the neighbourhood of the self-dual line, the diverging inverse wave vector defines the most relevant length scale.

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