Spin Operator Matrix Elements in the Superintegrable Chiral Potts Quantum Chain

N. Iorgov · S. Pakuliak · V. Shadura · Y. Tykhyy · G. von Gehlen

Abstract We derive spin operator matrix elements between general eigenstates of the superintegrable $\mathbb{Z}_N$-symmetric chiral Potts quantum chain of finite length. Our starting point is the extended Onsager algebra recently proposed by Baxter. For each pair of spaces (Onsager sectors) of the irreducible representations of the Onsager algebra, we calculate the spin matrix elements between the eigenstates of the Hamiltonian of the quantum chain in factorized form, up to an overall scalar factor. This factor is known for the ground state Onsager sectors. For the matrix elements between the ground states of these sectors we perform the thermodynamic limit and obtain the formula for the order parameters. For the Ising quantum chain in a transverse field ($N = 2$ case) the factorized form for the matrix elements coincides with the corresponding expressions obtained recently by the Separation of Variables method.

Keywords Quantum integrable spin chain · Chiral Potts model · Order parameter · Onsager algebra

1 Introduction

The solution of the Ising model by Onsager [1] in 1944 was a major breakthrough in mathematical physics. The subsequent calculation of the Ising magnetization by Yang [2] in 1952

N. Iorgov · V. Shadura · Y. Tykhyy
Bogolyubov Institute for Theoretical Physics, Kiev 03143, Ukraine

N. Iorgov
e-mail: iorgov@bitp.kiev.ua

S. Pakuliak
Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141980, Moscow region, Russia
e-mail: pakuliak@theor.jinr.ru

G. von Gehlen (✉)
Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany
e-mail: gehlen@th.physik.uni-bonn.de

(after the announcement of the formula by Onsager [3] in 1949) was an achievement of similar importance. The main tool in Onsager's work [1] was the introduction of the algebra which now carries his name. Later many alternative methods for solving the Ising model were invented and the interest in Onsager's algebra faded away. It was not revived until 1985 when the superintegrable chiral Potts quantum chain (SCPC) was formulated [4]. For more than 40 years the Ising model had remained the only known representation of Onsager's algebra. Then the SCPC provided a whole series of new Onsager algebra representations. In many respects, the SCPC is the $\mathbb{Z}_N$ generalization of the $\mathbb{Z}_2$ Ising model. Soon, in 1988, Baxter [5] calculated the partition function of the SCPC, using functional relations of the 2-dimensional integrable chiral Potts model [6, 7]. The formula for the order parameter of the SCPC (the generalization of the famous Onsager–Yang result for the Ising model) was conjectured slightly earlier in 1988 by Albertini-McCoy-Perk-Tang [8] from a perturbative calculation up to k'^5 for arbitrary N (see also [9]). However, it took until 2005 that Baxter [10, 11] succeeded to prove the conjectured formula. His derivation used functional relations for the τ_2-model and natural analytical assumptions.

Nevertheless, Baxter [12] insisted that a purely algebraic derivation of the order parameter formula would be desirable. So, recently, he extended the Onsager algebra by a SCPC-spin operator [13]. One has to include many new operators which are produced by commutations with the generators of the Onsager algebra. R. Baxter conjectured that the two simplest relations in the extended Onsager algebra uniquely define (up to a common multiplier) the matrix elements of the spin operator between vectors from the ground state Onsager sectors. Recently he proved that this conjecture implies the determinant representation [14] and obtained, in the thermodynamic limit, the formula for the order parameters [15].

Our starting point for this research was that we compared Baxter's conjectured equation (3.45) of [13] to the factorized formula (78) in [16] for the Ising quantum chain spin operator matrix elements which we had obtained by the method of Separation of Variables. In the case of the Ising chain, after a simple transformation given in Sect. 4.1 of the present paper, (3.45) of [13] should imply (78) of [16]. Since Baxter's conjecture was formulated for the arbitrary parameters, it was natural to suggest that the factorized formula (78) in [16] for the ground Onsager sectors is valid also for the ground Onsager sectors in SCPC if one uses appropriate parameters labelling these sectors. Numerical calculations for the finite length chain together with calculations for the thermodynamic limit (see Appendix C) strongly supported our conjecture. This encouraged us to prove the Baxter's conjecture (3.45) from [13].

In the present paper we generalize this conjecture to arbitrary Onsager sectors and prove it. We found that the matrix elements of spin operators between the eigenvectors of the SCPC Hamiltonian for arbitrary Onsager sectors can be presented in a factorized form. The problem of finding the matrix elements of the spin operator is reduced to the problem of finding non-zero matrix elements of the spin operator between some particular vectors from the corresponding two irreducible representations of the Onsager algebra. In the case of ground state Onsager sectors this gives an exact factorized formula for the matrix elements of spin operators between such type eigenvectors. Finally, taking the thermodynamic limit of ground states matrix elements, we derive the Albertini et al. formula [8, 9] for the order parameters. We would like to note that factorized formulas for the spin matrix elements exist also for the 2D Ising model [17] and for the quantum XY-chain [18].

Recently, state vectors for the superintegrable chiral Potts model were investigated exploiting the $sl(2)$-loop algebra symmetry of the τ_2-model [19, 20], which is closely related to the chiral Potts model [21–26]. Since our approach avoids direct use of the relation to the τ_2-model, we shall not go into details of this exciting work.

This paper is organized as follows: In Sect. 2 we define the SCPC by its Hamiltonian and use the fact that its two parts generate the Onsager algebra and imply the Ising form of the eigenvalues. Baxter's extension and the basic two resulting equations for the spin operator are stated. In Sect. 3 we develop the consequences of Baxter's two equations for spin matrix elements: including higher Onsager sectors and in several steps fixing the explicit solution. Specializing to the ground state sector, we show that our result coincides with Baxter's conjecture. The section ends with the discussion of some non-trivial selection rules for the spin matrix elements. In Sect. 4 we sandwich the expression for the spin operator between eigenvectors of the Hamiltonian. The sum over the intermediate labels is performed explicitly, resulting in fully factorized expressions. Finally, performing the thermodynamic limit in Sect. 5, the formula for the order parameters is obtained. Section 6 summarizes our results. Technical details about performing the factorization and the thermodynamic limit are given in Appendices A–C, together with a numerical example.

2 The Superintegrable Chiral Potts Quantum Chain

2.1 The Hamiltonian of the Superintegrable Chiral Potts Quantum Chain

The superintegrable $\mathbb{Z}_N$-symmetric chiral Potts quantum chain of length L is defined by the Hamiltonian [4]

$$\mathcal{H} = \mathcal{H}_0 + \mathsf{k}'\mathcal{H}_1, \tag{1}$$

where k' is a temperature-like real parameter, $\omega = e^{2\pi i/N}$, $N \in \mathbb{Z}$, $N \geq 2$, and

$$\mathcal{H}_0 = -2 \sum_{j=1}^{L} \sum_{n=1}^{N-1} \frac{Z_j^n Z_{j+1}^{-n}}{1 - \omega^{-n}}, \qquad \mathcal{H}_1 = -2 \sum_{j=1}^{L} \sum_{n=1}^{N-1} \frac{X_j^n}{1 - \omega^{-n}}. \tag{2}$$

The space of states is the L-fold tensor product of spaces $\mathbb{C}^N$ at each site j. The operators $Z_j, X_j \in \mathrm{End}\,(\mathbb{C}^N)^{\otimes L}$ act non-trivially only at site j:

$$Z_j = \mathbf{1} \otimes \cdots \otimes \mathbf{1} \otimes \underbrace{Z}_{j\text{-th}} \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1},$$

$$X_j = \mathbf{1} \otimes \cdots \otimes \mathbf{1} \otimes \underbrace{X}_{j\text{-th}} \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1}.$$

Z and X are the $\mathbb{Z}_N$-generalizations of the $\mathbb{Z}_2$-Pauli operators σ_z and σ_x. They satisfy the Weyl relation $ZX = \omega XZ$ and $Z^N = X^N = \mathbf{1}$. We always take periodic boundary conditions $Z_{L+1} = Z_1$. A convenient representation is to label the state vectors by spin variables $\sigma_j \in \mathbb{Z}_N$, $j = 1, \ldots, L$, writing the state vectors as $|\sigma_1, \sigma_2, \ldots, \sigma_L\rangle$ and

$$(Z_j)_{\sigma_j, \sigma_j'} = \delta_{\sigma_j, \sigma_j'} \omega^{\sigma_j}, \qquad (X_j)_{\sigma_j, \sigma_j'} = \delta_{\sigma_j, \sigma_j'+1}. \tag{3}$$

Both $\mathcal{H}_0$ and $\mathcal{H}_1$ commute with the spin rotation operator $R = X_1 X_2, \ldots, X_L$. Since $R^N = 1$, the space of states of SCPC decomposes into sectors of fixed of $\mathbb{Z}_N$-charge Q where $Q = 0, 1, \ldots, N - 1$, corresponding to the eigenvalues ω^Q of the R.

It turns out [27] that for $N = 3$ and $0 \leq \mathsf{k}' < 0.901\ldots$ we are in the ferromagnetic regime, where in the thermodynamic limit the system acquires a non-zero value of the order parameters. One aim of this paper is to derive its value as a function of k'.

The Hamiltonian (1) can be derived as a logarithmic derivative with respect to a rapidity parameter from the homogeneous 2D superintegrable chiral Potts model. However, we shall avoid using properties of the two-dimensional model.

2.2 The Onsager Algebra and the Superintegrable Chiral Potts Quantum Chain

In the beginning of the 1980'th chiral Potts quantum chains received much attention since for certain parameter values they exhibit an incommensurate phase. Since no chain of this class was known to be integrable, Howes, Kadanoff and den Nijs [28] studied perturbative expansions. They found strong evidence that the $\mathbb{Z}_3$ version of (1) has a terminating low-temperature expansion for the mass gap. Subsequent numerical studies in [4] showed: if in the $\mathbb{Z}_N$-symmetric quantum chain the coefficients of the terms involving $Z_j Z_{j+1}$ and X_j are chosen as in (2), many gaps become linear. This feature is known from the Ising model and motivated further studies of the Hamiltonian (1), (2). Now is was known that Hamiltonians of the form $\mathcal{H} \sim A_0 + \mathsf{k}' A_1$ are integrable if A_0 and A_1 satisfy the Dolan-Grady-relations [29]

$$\left[A_j, \left[A_j, \left[A_j, A_{1-j}\right]\right]\right] = 16\left[A_j, A_{1-j}\right], \quad j = 0, 1. \tag{4}$$

Indeed, in [4] it was shown that, putting

$$A_0 = -2\mathcal{H}_1/N, \qquad A_1 = 2\mathcal{H}_0/N$$

the relations (4) are satisfied. As has first been pointed out by Perk [30], a pair of operators A_0, A_1 satisfying (4) generates a basis of Onsager's infinite dimensional Lie-algebra with the operators $A_m, m \in \mathbb{Z}, G_n, n \in \mathbb{N}$:

$$\begin{aligned}
[A_m, A_n] &= 4G_{m-n}, \qquad G_{-n} = -G_n, \\
[G_m, A_n] &= 2A_{m+n} - 2A_{n-m}, \qquad [G_m, G_n] = 0.
\end{aligned} \tag{5}$$

The study of the representation theory of the Onsager algebra has been started by Davies [31]. He showed that certain finite-dimensional representations of the Onsager algebra are related to representations of a direct sum of several copies of the Lie algebra $sl(2)$, see also [32–34]. In the case of the SCPC only two-dimensional representations of $sl(2)$ appear. Unlike the $N = 2$ Ising case, for $N \geq 3$ the Onsager algebra alone is not powerful enough to fully determine the eigenvalues. However, in each Onsager sector of the SCPC the 2^{m_E} eigenvalues of $\mathcal{H}$ have the Ising-like form

$$E = A + \mathsf{k}'B - N \sum_{j=1}^{m_E} \pm\varepsilon(\theta_j), \tag{6}$$

with

$$\varepsilon(\theta) = \sqrt{1 - 2\mathsf{k}'\cos\theta + \mathsf{k}'^2}. \tag{7}$$

The constants A and B and the m_E values θ_j label irreducible representations of the Onsager algebra.

Using functional relations which follow from the general integrable 2-dimensional chiral Potts model [20], or, recently, exploiting the loop symmetry of the related τ_2-model [21], the θ_j can be calculated from the zeros of the Baxter-Albertini-McCoy-Perk (BAMP) polynomials [5, 35, 36]. However, here we shall follow the spirit of Baxter's recent work and

determine the spin-operator matrix elements from the Onsager algebra and an extension of this algebra alone. So, the θ_j will be considered as free parameters. Of course, specific values of the θ_j calculated from the zeros of the BAMP-polynomials may be inserted in the final formulas.

2.3 Extension of the Onsager Algebra by a Spin Operator

In [13] Baxter considered commutators of $\mathcal{H}_0$ and $\mathcal{H}_1$ with the local spin operator $S = Z_1^r$ where r may be chosen to take the values $r = 1, \ldots, N-1$ (because of the periodic boundary conditions we may choose the site index 1). He introduced two operations on operators X in the space of states

$$f_0(X) = \frac{[\mathcal{H}_0, X]}{2N}, \quad \text{and} \quad f_1(X) = \frac{[\mathcal{H}_1, X] + 2rX}{2N} \tag{8}$$

and has shown that

$$f_0(S) = 0, \quad \text{and} \quad f_1(f_1(S)) = f_1(S). \tag{9}$$

Repeated commutation of S with $\mathcal{H}_0$ and $\mathcal{H}_1$ produces many new elements. However, Baxter made the conjecture that in the case when the finite-dimensional representations of Onsager algebra are related to two-dimensional representations of $sl(2)$ (in particular, in the case of SCPC) already the mentioned two relations for S uniquely (up to a multiplier because the relations are homogeneous) define the matrix elements of S. In the following section we prove this conjecture.

3 Conjecture on the Reduced Matrix S_{PQ}: a Generalization, Reformulation and a Proof

3.1 Generalization

We consider the restrictions of the Hamiltonian $\mathcal{H}$ to the subspaces which are spaces of irreducible representations of the Onsager algebra. We shall call these subspaces *Onsager Sectors*. Let $\mathcal{V}^P$, $\mathcal{V}^Q$ be some Onsager sectors with $\mathbb{Z}_N$-charges P, Q and dimensions $2^{m_E^P}$, $2^{m_E^Q}$, respectively. We will use the short notations $m = m_E^P$, $n = m_E^Q$. From [22, 31, 36] we know that on such a subspace, the restricted Hamiltonian $H_{\mathcal{V}^P}$ has an Ising-like spectrum of the form (6), (7).

Now we write a Hamiltonian $H_{\mathcal{V}^P}$ (we shall use the short notation H^P), which has the eigenvalues (6), (7):

$$H^P = H_0^P + \mathsf{k}' H_1^P, \quad H_0^P = A^P - N F_0^P, \quad H_1^P = B^P + N F_1^P, \tag{10}$$

where A^P and B^P are some constants depending on this Onsager sector and

$$F_0^P = \sum_{j=1}^{m} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j, \qquad F_1^P = \sum_{j=1}^{m} \begin{pmatrix} \cos\theta_j & \sin\theta_j \\ \sin\theta_j & -\cos\theta_j \end{pmatrix}_j. \tag{11}$$

We write analogous formulas for the sector $\mathcal{V}^Q$ with charge Q and with parameters θ'_j, $j = 1, 2, \ldots, n$:

$$F_0^Q = \sum_{j=1}^n \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j, \qquad F_1^Q = \sum_{j=1}^n \begin{pmatrix} \cos\theta'_j & \sin\theta'_j \\ \sin\theta'_j & -\cos\theta'_j \end{pmatrix}_j. \tag{12}$$

Using the fact that $\mathcal{H}_0$ and $\mathcal{H}_1$ are block-diagonal with respect to irreducible representations of the Onsager algebra and taking the formulas (8) between arbitrary states from $\mathcal{V}^P$ and $\mathcal{V}^Q$, we obtain

$$f_0(X_{PQ}) = -\frac{1}{2}(F_0^P X_{PQ} - X_{PQ} F_0^Q + \alpha X_{PQ}), \tag{13}$$

$$f_1(X_{PQ}) = \frac{1}{2}(F_1^P X_{PQ} - X_{PQ} F_1^Q + (\beta + 1)X_{PQ}), \tag{14}$$

where X_{PQ} is a rectangular submatrix in X and

$$\alpha = (A^Q - A^P)/N, \qquad \beta = (B^P - B^Q + 2r - N)/N, \tag{15}$$

and we define $r = Q - P$ for $P < Q$ and $r = Q - P + N$ for $P > Q$. The corresponding eigenvectors of H^P, H^Q are easily obtained and will be given in (55)–(57).

We are interested in matrix elements of the spin operator $S = Z_1^r$. In the basis of distinct Onsager irreps S is a block matrix. Since S changes the $\mathbb{Z}_N$-charge, it has vanishing diagonal blocks, but it can have non-zero blocks between spaces $\mathcal{V}^P$ and $\mathcal{V}^Q$ of equal or different dimensions 2^m and 2^n. So, in general, one particular submatrix (block) S_{PQ} will be a rectangular $2^m \times 2^n$-matrix.

From (9), (13)–(15) decomposed into Onsager sectors, the submatrix S_{PQ} will be proportional to a solution C of the pair of equations

$$F_0^P C - C F_0^Q + \alpha C = 0, \tag{16}$$

$$F_1^P F_1^P C - 2F_1^P C F_1^Q + C F_1^Q F_1^Q + 2\beta(F_1^P C - C F_1^Q) + (\beta^2 - 1)C = 0. \tag{17}$$

The F_0^P, F_0^Q, F_1^P, F_1^Q are given above and α, β are supposed to be arbitrary constants. Formulas (13), (14), (16), (17) generalize Baxter's relations from [13] which were written only for ground state Onsager sectors.

The system of (16), (17) is homogeneous and any solution of this system multiplied by a constant is also a solution. We will find a solution C_{PQ} of the system (16), (17) and show that the space of solutions is no more than one-dimensional. Therefore *exact*[1] matrix elements S_{PQ} of the spin operator $S = Z_1^r$ are related to this solution by the relation $S_{PQ} = \mathcal{N}_{PQ}C_{PQ}$ with an unknown scalar multiplier $\mathcal{N}_{PQ}$, which should be fixed from other arguments. The other relations of the extended Onsager algebra do not spoil the equality $S_{PQ} = \mathcal{N}_{PQ}C_{PQ}$, but they may impose that $\mathcal{N}_{PQ} = 0$.

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[1] In the following the term "exact matrix elements" will be used in the sense that the constants $\mathcal{N}_{PQ}$ have been determined too.

3.2 Reformulation

Multiplying the relations (16), (17) from the right by

$$G = \prod_{j=1}^{n} \sigma_j^x \sigma_j^z, \tag{18}$$

using $F_0^Q = -G^{-1}F_0^Q G$, $F_1^Q = -G^{-1}F_1^Q G$ and denoting $\tilde{C} = CG$, we get similar relations but with changed signs at F_0^Q and F_1^Q:

$$F_0^P \tilde{C} + \tilde{C} F_0^Q + \alpha \tilde{C} = 0, \tag{19}$$

$$F_1^P F_1^P \tilde{C} + 2F_1^P \tilde{C} F_1^Q + \tilde{C} F_1^Q F_1^Q + 2\beta(F_1^P \tilde{C} + \tilde{C} F_1^Q) + (\beta^2 - 1)\tilde{C} = 0. \tag{20}$$

Let us combine the matrix elements $\tilde{C}_{\gamma,\beta}$ into a vector $\tilde{K} \in \mathcal{V}^P \otimes \mathcal{V}^Q$ with components $\tilde{K}_{(\gamma,\beta)}$ labelled by multi-indices. The vector $\tilde{K}$ has dimension 2^μ, where $\mu = m + n$. Let for $k = 0, 1$

$$F_k = F_k^P \otimes \mathbf{1} + \mathbf{1} \otimes (F_k^Q)^t \tag{21}$$

be an operator in $\mathcal{V}^P \otimes \mathcal{V}^Q$ and $(F_k^Q)^t$ is the transposition of F_k^Q. Then the relations (19) and (20) become

$$(F_0 + \alpha)\tilde{K} = 0, \qquad (F_1 + \beta - 1)(F_1 + \beta + 1)\tilde{K} = 0. \tag{22}$$

This procedure puts the parameters $\{\theta_j\}$ and $\{\theta_j'\}$ on an equal footing: we combine these two sets into the set

$$\{\vartheta_1, \ldots, \vartheta_\mu\} = \{\theta_1, \ldots, \theta_m, \theta_1', \ldots, \theta_n'\}. \tag{23}$$

Since the matrices F_0 and F_1 are both traceless with determinant -1 we can find a similarity transformation $F_1 = \tilde{U}^{-1} F_0 \tilde{U}$ to get

$$(F_0 + \beta - 1)(F_0 + \beta + 1)\tilde{U}\tilde{K} = 0, \tag{24}$$

where

$$\tilde{U} = UU_d, \quad U = \prod_{j=1}^{\mu} \begin{pmatrix} \cos\vartheta_j + 1 & \cos\vartheta_j - 1 \\ 1 & 1 \end{pmatrix}_j, \quad U_d = \prod_{j=1}^{\mu} \begin{pmatrix} 1 & 0 \\ 0 & -\cot(\vartheta_j/2) \end{pmatrix}_j. \tag{25}$$

It gives finally two relations for the vector $K = U_d \tilde{K}$:

$$(F_0 + \alpha)K = 0, \qquad (F_0 + \beta - 1)(F_0 + \beta + 1)UK = 0, \tag{26}$$

where we use the fact that F_0 commutes with U_d. In the next two subsections we will solve the system of (26) with respect to K for arbitrary parameters α, β.

3.3 Number of Solutions of (26)

The relations (26) are a system of linear homogeneous equations with respect to the un-
known components of K. In this subsection we estimate the number of solutions of this
system, depending on α and β. We use the notation $F = F_0$.

Theorem 1 *The dimension of the space of solutions K of the system*

$$(F + \alpha)K = 0, \tag{27}$$

$$(F + \beta - 1)(F + \beta + 1)UK = 0, \tag{28}$$

where

$$F = \sum_{j=1}^{\mu} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j, \qquad U = \prod_{j=1}^{\mu} \begin{pmatrix} c_j + 1 & c_j - 1 \\ 1 & 1 \end{pmatrix}_j \tag{29}$$

*at generic values of the parameters $c_k = \cos \vartheta_k$, $k = 1, \ldots, \mu$, is no more than one-
dimensional. It is one-dimensional if and only if*

- μ *is even, $\alpha = 0$, $\beta = \pm 1$,* \tag{30}

- μ *is odd, $\alpha = \pm 1$, $\beta = 0$.* \tag{31}

Proof The spectrum of F is $\mu, \mu - 2, \ldots, -\mu$. From the first relation (27) we have a nec-
essary restriction on α in order to have $K \neq 0$: *α should be an integer of the same parity
as μ, and $|\alpha| \leq \mu$*. If α satisfies this condition, the space of solutions of (27) has dimen-
sion $\binom{\mu}{(\mu+\alpha)/2}$. The second relation (28) requires the existence of such K from this subspace
which are annihilated by the operator $(F + \beta - 1)(F + \beta + 1)U$. Thus, to have $K \neq 0$, *$\mu + \beta$
should be an odd integer and $|\beta| \leq \mu + 1$*. Otherwise, since U is invertible, we would have
that $(F + \beta - 1)(F + \beta + 1)U$ is also invertible and therefore $K = 0$.

We will prove the theorem by induction over μ. Let $F = F_{(\mu)}$ be the initial matrix. In a
basis in which the μ-th tensor component is separated, we have

$$F_{(\mu)} + \alpha = F_{(\mu-1)} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_\mu + \alpha = \begin{pmatrix} F_{(\mu-1)} + \alpha + 1 & 0 \\ 0 & F_{(\mu-1)} + \alpha - 1 \end{pmatrix}.$$

It is a diagonal matrix and the zeros on its diagonal define the space of solutions of (27). Let
$\mathcal{P}_{(\mu)}(\alpha)$ be the projector to this subspace. Its rank is

$$\text{rk}\,\mathcal{P}_{(\mu)}(\alpha) = \binom{\mu}{(\mu+\alpha)/2}.$$

In the basis with separated μ-th tensor component this projector is

$$\mathcal{P}_{(\mu)}(\alpha) = \begin{pmatrix} \mathcal{P}_{(\mu-1)}(\alpha + 1) & 0 \\ 0 & \mathcal{P}_{(\mu-1)}(\alpha - 1) \end{pmatrix}.$$

We need to calculate the rank

$$f(\mu, \alpha, \beta) = \text{rk}\left((F_{(\mu)} + \beta - 1)(F_{(\mu)} + \beta + 1)U_{(\mu)}\mathcal{P}_{(\mu)}(\alpha)\right),$$

since the difference

$$\tilde{f}(\mu, \alpha, \beta) = \mathrm{rk}\,\mathcal{P}_{(\mu)}(\alpha) - f(\mu, \alpha, \beta) \geq 0$$

defines the dimension of the space of solutions of the system of (27) and (28).

Extracting explicitly the μ-th tensor component we have

$$f(\mu, \alpha, \beta) = \mathrm{rk}\begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

where

$$A = (c_\mu + 1)(F_{(\mu-1)} + \beta + 2)(F_{(\mu-1)} + \beta)U_{(\mu-1)}\mathcal{P}_{(\mu-1)}(\alpha + 1),$$

$$B = (c_\mu - 1)(F_{(\mu-1)} + \beta + 2)(F_{(\mu-1)} + \beta)U_{(\mu-1)}\mathcal{P}_{(\mu-1)}(\alpha - 1),$$

$$C = (F_{(\mu-1)} + \beta)(F_{(\mu-1)} + \beta - 2)U_{(\mu-1)}\mathcal{P}_{(\mu-1)}(\alpha + 1),$$

$$D = (F_{(\mu-1)} + \beta)(F_{(\mu-1)} + \beta - 2)U_{(\mu-1)}\mathcal{P}_{(\mu-1)}(\alpha - 1).$$

By $f(\mu, \alpha, \beta)$ we denote the rank which is calculated at generic values of the parameters c_k, $k = 1, \ldots, \mu$. At some specific values of these parameters, the corresponding rank may be smaller than at generic values. At $c_\mu = 1$ we have $B = 0$ and using the fact that the rank of a block-triangular matrix is greater or equal to the sum of ranks of diagonal blocks we obtain

$$f(\mu, \alpha, \beta) \geq \mathrm{rk}A + \mathrm{rk}D = f(\mu - 1, \alpha + 1, \beta + 1) + f(\mu - 1, \alpha - 1, \beta - 1). \tag{32}$$

Similarly, at $c_\mu = -1$ we have $A = 0$ and

$$f(\mu, \alpha, \beta) \geq \mathrm{rk}B + \mathrm{rk}C = f(\mu - 1, \alpha - 1, \beta + 1) + f(\mu - 1, \alpha + 1, \beta - 1). \tag{33}$$

Using identities between binomial coefficients, the inequalities (32) and (33) become

$$\tilde{f}(\mu, \alpha, \beta) \leq \tilde{f}(\mu - 1, \alpha + 1, \beta + 1) + \tilde{f}(\mu - 1, \alpha - 1, \beta - 1), \tag{34}$$

$$\tilde{f}(\mu, \alpha, \beta) \leq \tilde{f}(\mu - 1, \alpha - 1, \beta + 1) + \tilde{f}(\mu - 1, \alpha + 1, \beta - 1). \tag{35}$$

We now show by induction in μ that

$$\tilde{f}(\mu, \alpha, \beta) \leq \delta_{\alpha^2 + \beta^2, 1}. \tag{36}$$

Assuming that the binomial coefficients $\binom{k}{l}$ are defined to be 0 if $l < 0$ or $l > k$, we can start the induction from the case $\mu = 1$ and arbitrary α, β. In this case, as it has been explained in the beginning of the proof, in order to have $K \neq 0$ we need to choose $\alpha = \pm 1$ and $\beta \in \{-2, 0, 2\}$. Let for definiteness $\alpha = 1$. Then

$$f(1, \alpha, \beta) = \mathrm{rk}\left((F_{(1)} + \beta - 1)(F_{(1)} + \beta + 1)U_{(1)}\mathcal{P}_{(1)}(\alpha)\right)$$

$$= \begin{pmatrix} (\beta + 2)\beta & 0 \\ 0 & \beta(\beta - 2) \end{pmatrix} U \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{37}$$

If $\beta = 0$ then $f(1, \alpha, \beta) = 0$, otherwise $f(1, \alpha, \beta) = 1$. Thus only if $\beta = 0$ we have $\tilde{f}(1, \alpha, \beta) = 1$.

Then we assume $\tilde{f}(\mu - 1, \alpha, \beta) \leq \delta_{\alpha^2 + \beta^2, 1}$, and straightforward analysis shows that the inequalities (34), (35) imply (36), completing the induction.

This proves that the space of solutions K is no more than one-dimensional if α and β satisfy the relations (30) or (31). Otherwise there is only the trivial solution $K = 0$. In the next subsection we give the explicit solution for K if α and β satisfy (30) or (31). It proves that in these cases the space of solutions is one-dimensional. □

What is the condition on the parameters c_k, $k = 1, \ldots, \mu$, which leads the theorem to fail? The analysis for $\mu \leq 3$ gives that this condition is: either $c_1 = c_2 = c_3$, or a pair of c_k coincide with $+1$ (or -1).

If both $\mathcal{V}^P$ and $\mathcal{V}^Q$ are ground state Onsager sectors, the θ_k, θ'_k are determined by the zeros of the ground state (i.e. with no Bethe excitations) BAMP-polynomials. For any L these zeros are determined from the intersection of two simple curves [40]. From the behavior of these curves it is easy to show that the c_k and c'_k cannot coincide or reach ± 1. So, e.g. for the calculation of the order parameter, we are on the save side. For higher Onsager sectors (which are also included in our consideration here) the situation is not easy, as the solutions of Bethe-type equations enter the determination of the zeros. Here we can just conjecture that for general μ, the corresponding condition is too restrictive and the sets c_k arising in the SCPC will not satisfy the above condition.

3.4 The Solution for the Matrix Elements

In the last subsection we proved that if a non-trivial solution K exists, then it is unique up to a multiplier. If μ is even, such a solution exists iff $\alpha = 0$ and $\beta = \pm 1$, if μ is odd, then iff $\alpha = \pm 1$ and $\beta = 0$.

We now present the solution K in the basis of eigenvectors of F. Each basis vector is a tensor product of the two-dimensional vectors associated with summands of F in (29). We label each basis vector by the subset I of the set $\{1, 2, \ldots, \mu\}$, such that the elements of I label the tensor components where the two-dimensional basis vectors with the eigenvalue $+1$ are located. The complementary subset $\bar{I}$ contains the labels of the tensor components where the two-dimensional basis vectors with the eigenvalue -1 are placed. By $|I|$ we denote the size of the subset I.

We use a short notation: the product of an expression containing the variable c indexed by a subset I means the product of this expression over the elements of the subset with variable c indexed by the elements of I, e.g.

$$\prod (c_I - c_{\bar{I}}) = \prod_{j \in I} \prod_{k \in \bar{I}} (c_j - c_k). \tag{38}$$

Recall that $j \in I$ iff the component j of the product eigenvector F (29) belongs to the eigenvalue $+1$, otherwise it is in $\bar{I}$. F combines the left-hand state vectors of $\mathcal{V}^P$ in its first m components with the right-hand vectors $\mathcal{V}^Q$ in its last n components, see (21). So c_j will stand for $\cos \theta_j$ if $j \leq m$ and for $\cos \theta'_{j-m}$ for $m < j \leq n + m$, see (23). Because of the conjugation performed by G in (18), the sign of the eigenvalues in $\mathcal{V}^Q$ is opposite to the sign of the eigenvalues in F.

Theorem 2 *Let the parameters α and β satisfy* (30) *or* (31). *The vector K with the components*

$$K_I = \frac{\delta_{|I|,(\mu-\alpha)/2}}{\prod (c_I - c_{\bar{I}}) \prod (c_I + 1)^\sigma \prod (c_{\bar{I}} - 1)^\tau} \tag{39}$$

is the unique (*up to a scalar multiplier*) *solution of the system* (27) *and* (28). *Here*

$$\sigma = (\beta - \alpha + 1)/2, \qquad \tau = (\beta + \alpha + 1)/2. \tag{40}$$

Remark Due to the special values of α and β, each of σ and τ can be either 0 or 1.

Proof The numerator $\delta_{|I|,(\mu-\alpha)/2}$ ensures that K satisfies (27).

Let us prove that K satisfies (28). In fact we need to prove that the non-zero components of $M = UK$ are in the eigenspaces of F with eigenvalues $-\beta - 1$ and $-\beta + 1$. The components of the vector $M = UK$ are

$$M_J = \sum_I U_{J,I} K_I = \sum_I \frac{\prod(c_{I\cap J} + 1)\prod(c_{\bar{I}\cap J} - 1)\delta_{|I|,(\mu-\alpha)/2}}{\prod(c_I - c_{\bar{I}})\prod(c_I + 1)^\sigma \prod(c_{\bar{I}} - 1)^\tau}, \tag{41}$$

where we used $U_{J,I} = \prod(c_{I\cap J} + 1)\prod(c_{\bar{I}\cap J} - 1)$ which follows from (29). The components of M are

$$M_J = \frac{P}{\prod(c_J - c_{\bar{J}})\prod(c_J + 1)^\sigma \prod(c_{\bar{J}} - 1)^\tau} \tag{42}$$

with an unknown polynomial P in the numerator. Let us explain the origin of the different factors in the denominator of (42). First, there are no factors like $c_j + 1$, $j \in J$ in the denominator of (42), because all such factors with $j \in I$ in the denominator of (41) are cancelled. Similarly, there are no factors like $c_j - 1$, $j \in J$. Second, there are no factors like $c_j - c_{j'}$, $j, j' \in J$, in the denominator of (42). Potentially such factors can arise from summands in (41) for which $j \in I$ and $j' \in \bar{I}$. But to each such summand there corresponds a summand with I replaced by $\tilde{I} = \{j'\} \cup I \backslash \{j\}$. A straightforward analysis shows that the sum of these two summands does not contain a pole at $c_j = c_{j'}$. Similarly there are no factors like $c_j - c_{j'}$, $j, j' \in \bar{J}$ in the denominator of (42).

Let us estimate the degree of P with respect to the variables c_j, $j \in J$. It is

$$\max(1 - \sigma - |\bar{I}|, 1 - \tau - |I|) + |\bar{J}| \geq \deg P \geq 0.$$

The two arguments of the maximum correspond to the fact that each element of J is either in I or in $\bar{I}$. The term $|\bar{J}|$ corresponds to the denominator of (42). Similarly, the estimate of the degree of P with respect to the variables c_j, $j \in \bar{J}$, gives

$$\max(-\sigma - |\bar{I}|, -\tau - |I|) + |J| + \sigma + \tau \geq \deg P \geq 0.$$

In order to get $M = UK \neq 0$ both inequalities have to be satisfied. Using $|I| = (\mu - \alpha)/2$, $|\bar{I}| = (\mu + \alpha)/2$, these give

$$|\bar{J}| \geq (\mu + \beta - 1)/2, \qquad |J| \geq (\mu - \beta - 1)/2.$$

Since $|J| + |\bar{J}| = \mu$ there are only two possibilities: $|J| = (\mu - \beta - 1)/2$, $|\bar{J}| = (\mu + \beta + 1)/2$ or $|J| = (\mu - \beta + 1)/2$, $|\bar{J}| = (\mu + \beta - 1)/2$. The corresponding eigenvalue $|J| - |\bar{J}|$ of F is $-\beta - 1$ or $-\beta + 1$, respectively. It means that K satisfies (28). The theorem is proved.   □

In order to obtain matrix elements of $S = Z_1^r$ between the states from Onsager sectors we need to rewrite the solution K given by (39) in the original notations.

We will label each basis vector in $\mathcal{V}^P$ by the subset V of the set $\{1, 2, \ldots, m\}$ corresponding to the tensor components where the two-dimensional basis vectors with the eigenvalue $+1$ of F_0^P are located. The complementary subset W contains the labels of the tensor components for which the two-dimensional basis vectors with the eigenvalue -1 are placed. In the same way we define the subsets V' and W' of the set $\{1, 2, \ldots, n\}$ to label the basis vectors in the space $\mathcal{V}^Q$.

We also use the set of indices $\{1, 2, \ldots, m+n\}$. We will identify the indices $\{1, 2, \ldots, m\}$ with indices of tensor components of $\mathcal{V}^P$. The rest indices $\{m+1, m+2, \ldots, m+n\}$ of the set $\{1, 2, \ldots, m+n\}$ are identified with indices $\{1, 2, \ldots, n\}$ of tensor components of $\mathcal{V}^Q$ by subtraction m. This identification defines a one to one correspondence between the subsets in $\{1, 2, \ldots, m+n\}$ with pairs of subsets from the sets $\{1, 2, \ldots, m\}$ and $\{1, 2, \ldots, n\}$.

Using the relation $\tilde{C} = CG$ with G defined in (18) and the relation $K = U_d \tilde{K}$ with U_d defined in (25) we have for the matrix element of C in the basis labeled by V and V'

$$
\begin{aligned}
C_{V,V'} &= (-1)^{|V'|} \tilde{C}_{V,W'} = (-1)^{|V'|} \tilde{K}_{(V,W')} \\
&= (-1)^{|W|} K_I \prod_{i \in W} \tan \theta_i / 2 \prod_{i \in V'} \tan \theta_i' / 2,
\end{aligned}
\tag{43}
$$

where $I = (V, W')$ is the subset in $\{1, 2, \ldots, m+n\}$ defined by the subsets V and W' according to the identification given above.

Note once more, that Theorem 2 defines the matrix elements $(C_{PQ})_{V,V'}$ by (43), (39) as solutions of the system of homogeneous equations (16) and (17). Exact matrix elements $(S_{PQ})_{V,V'}$ of the spin operator are given through the relation

$$
(S_{PQ})_{V,V'} = \mathcal{N}_{PQ} (C_{PQ})_{V,V'}
\tag{44}
$$

with an unknown constant $\mathcal{N}_{PQ}$ which depends on both Onsager sectors.

3.5 Matrix Elements Between Ground State Onsager Sectors

For the ground state Onsager sectors we have

$$
A^P = L(1-N) + Nm, \qquad A^Q = L(1-N) + Nn,
\tag{45}
$$

$$
B^P = 2P + L(1-N) + Nm, \qquad B^Q = 2Q + L(1-N) + Nn.
\tag{46}
$$

It was argued in [13] that in the *ground state* Onsager sectors one has $S_{V,V'} = 1$ for $W = \emptyset$, $W' = \emptyset$. In particular this relation defines exact values of the constants $\mathcal{N}_{PQ}$ for all pairs of ground state Onsager sectors.

Let us consider the case $P < Q, m$. Using (45), (46), (15) and (40) we obtain $\mu = 2m$, $\alpha = 0$, $\beta = -1$, $\sigma = \tau = 0$. The components (39) of K are

$$
K_I = \frac{\delta_{|I|,m}}{\prod (c_I - c_{\bar{I}})},
\tag{47}
$$

where c_I is the set $\{\cos \theta_i, \cos \theta_j'\}$, $i \in V$, $j \in W'$ and $c_{\bar{I}}$ is the set $\{\cos \theta_i, \cos \theta_j'\}$, $i \in W$, $j \in V'$. Recall that we are using a quite compact notation which was explained after (38). Because of the conjugation G in (18) we have to combine V with W' and V' with W.

Now using (43) and (47) we get $C_{V,V'}$. From the relations $S_{V,V'} = C_{V,V'} \mathcal{N}_{PQ}$ and $S_{V,V'} = 1$ for $W = \emptyset$, $W' = \emptyset$ we derive

$$\mathcal{N}_{PQ} = \frac{\prod_{i,j=1}^{m}(c_i - c'_j)}{\prod_{j=1}^{m} \tan \theta'_j/2}. \tag{48}$$

Thus our solution for $C_{V,V'}$ implies

$$S_{V,V'} = \delta_{|W|,|W'|} \prod_{i \in W} \tan \theta_i/2 \prod_{i \in W'} \cot \theta'_i/2$$
$$\times \frac{\prod_{i \in W, j \in V'}(c_i - c'_j) \prod_{i \in V, j \in W'}(c_i - c'_j)}{\prod_{i \in V, j \in W}(c_i - c_j) \prod_{i \in W', j \in V'}(c'_i - c'_j)}. \tag{49}$$

This formula for $S_{V,V'}$ coincides with the formula (45) conjectured by R. Baxter in [13] for the case $P < Q$, m. It means that Theorems 1 and 2 prove this conjecture.

Let us consider the case $P < Q$, $m + 1$. We have $\mu = 2m - 1$, $\alpha = -1$, $\beta = 0$, $\sigma = 1$, $\tau = 0$. In this case the components of K are

$$K_I = \frac{\delta_{|I|,m}}{\prod(c_I - c_{\bar{I}}) \prod(c_I + 1)}. \tag{50}$$

Now using (43) and (50) we get $C_{V,V'} = S_{V,V'} \mathcal{N}_{PQ}^{-1}$, where

$$S_{V,V'} = \delta_{|W|,|W'|} \prod_{i \in W} \sin \theta_i \prod_{i \in W'} (\sin \theta'_i)^{-1}$$
$$\times \frac{\prod_{i \in W, j \in V'}(c_i - c'_j) \prod_{i \in V, j \in W'}(c_i - c'_j)}{\prod_{i \in V, j \in W}(c_i - c_j) \prod_{i \in W', j \in V'}(c'_i - c'_j)}, \tag{51}$$

$$\mathcal{N}_{PQ} = \frac{\prod_{i=1}^{m}(1 + c_i) \cdot \prod_{i=1}^{m} \prod_{j=1}^{n}(c_i - c'_j)}{\prod_{i=1}^{n} \tan \theta'_i/2}. \tag{52}$$

This formula for $S_{V,V'}$ is again Baxter's formula in the case $P < Q$, $m + 1$.

We have also two other cases corresponding to $P > Q$ which can be considered analogously. In these cases our calculations also prove the Baxter's formula for $S_{V,V'}$. The first case is $P > Q$, m and we have $\mu = 2m$, $\alpha = 0$, $\beta = 1$, $\sigma = \tau = 1$,

$$\mathcal{N}_{PQ} = (-1)^m \prod_{i=1}^{m}(1 + c_i) \prod_{j=1}^{n} \sin \theta'_j \prod_{i=1}^{m} \prod_{j=1}^{n}(c_i - c'_j). \tag{53}$$

The second case is $P > Q$, $m - 1$ and we have $\mu = 2n - 1$, $\alpha = 1$, $\beta = 0$, $\sigma = 0$, $\tau = 1$,

$$\mathcal{N}_{PQ} = (-1)^n \prod_{j=1}^{n} \sin \theta'_j \prod_{i=1}^{m} \prod_{j=1}^{n}(c_i - c'_j). \tag{54}$$

3.6 Application: Selection Rules for Spin Matrix Elements

We proved that the non-trivial solution exists if and only if μ is even, $\alpha = 0$, $\beta = \pm 1$, or if μ is odd, $\alpha = \pm 1$, $\beta = 0$. This means that only in these cases we may have non-zero

matrix elements $S_{PQ} = \mathcal{N}_{PQ} C_{PQ}$ for spin operators. These selection rules are more fine than the selection rule by $\mathbb{Z}_N$-charge. They follow from (15). For $r = Q - P$ for $P < Q$, and $r = Q - P + N$ for $P > Q$ we have two cases where $C_{PQ} \neq 0$:

- $\mu = m + n$ is even and $A^Q - A^P = 0$, $B^P - B^Q = N \pm N - 2r$.
- $\mu = m + n$ is odd and $A^Q - A^P = \pm N$, $B^P - B^Q = N - 2r$.

   To be precise, these selection rules are not complete because the matrix elements for spin operators between vectors from two Onsager sectors were found up to a common multiplier $\mathcal{N}_{PQ}$. For a pair of specific Onsager sectors this multiplier can be zero even if $C_{PQ} \neq 0$. Additional information is needed whether $\mathcal{N}_{PQ}$ is zero or not.

   We have verified these selection rules numerically for $N = 3$, $L = 3$. In this case they are complete, that is all $\mathcal{N}_{PQ} \neq 0$ for the Onsager sectors defined by these selection rules.

4 Factorized Formula for Matrix Elements of Spin Operators for a Finite Chain

4.1 Matrix Elements of Spin Operators Between the eigenvectors of the Hamiltonian

As has been explained in Sect. 3.1, the Hamiltonian of the model restricted to the sector with charge P is

$$H^P = A^P + \mathsf{k}' B^P - N \sum_{j=1}^{m} \begin{pmatrix} 1 - \mathsf{k}' \cos \theta_j & -\mathsf{k}' \sin \theta_j \\ -\mathsf{k}' \sin \theta_j & -1 + \mathsf{k}' \cos \theta_j \end{pmatrix}_j.$$

The eigenvalues of H^P are

$$E = A^P + \mathsf{k}' B^P - N \sum_{j=1}^{m} \pm \varepsilon(\theta_j),$$

where

$$\varepsilon(\theta) = \sqrt{1 - 2\mathsf{k}' \cos \theta + \mathsf{k}'^2}, \qquad \varepsilon(0) = 1 - \mathsf{k}', \qquad \varepsilon(\pi) = 1 + \mathsf{k}'.$$

The $-\varepsilon(\theta_j)$ (resp. $+\varepsilon(\theta_j)$) in the sum corresponds to the presence (resp. absence) of the excitation with rapidity θ_j because the change $+\varepsilon(\theta_j)$ to $-\varepsilon(\theta_j)$ increases the energy. The eigenvector of H^P with the lowest energy (that is without excitations) is

$$\begin{pmatrix} a_0(\theta_1) \\ a_1(\theta_1) \end{pmatrix} \otimes \begin{pmatrix} a_0(\theta_2) \\ a_1(\theta_2) \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} a_0(\theta_m) \\ a_1(\theta_m) \end{pmatrix}, \tag{55}$$

$$a_0(\theta) = \frac{\mathsf{k}' \sin \theta}{\sqrt{\mathsf{k}'^2 \sin^2 \theta + (1 - \mathsf{k}' \cos \theta - \varepsilon(\theta))^2}},$$

$$a_1(\theta) = \frac{1 - \mathsf{k}' \cos \theta - \varepsilon(\theta)}{\sqrt{\mathsf{k}'^2 \sin^2 \theta + (1 - \mathsf{k}' \cos \theta - \varepsilon(\theta))^2}}, \tag{56}$$

with

$$a_0^2(\theta) + a_1^2(\theta) = 1.$$

It is useful to express the components $a_k(\theta_j)$, $k = 0, 1$, of the eigenvector through the energies $\varepsilon(\theta)$:

$$a_0(\theta) = \sqrt{\frac{(\varepsilon(\theta) + \varepsilon(0))(\varepsilon(\pi) + \varepsilon(\theta))}{4\varepsilon(\theta)}},$$

$$a_1(\theta) = -\sqrt{\frac{(\varepsilon(\theta) - \varepsilon(0))(\varepsilon(\pi) - \varepsilon(\theta))}{4\varepsilon(\theta)}}. \tag{57}$$

The formulas for the eigenvectors with some θ_j excited are obtained from the formula for the non-excited eigenvector by just replacing $\varepsilon(\theta_j) \to -\varepsilon(\theta_j)$ for all such θ_j. Therefore it is sufficient to consider matrix elements of the spin operator only between non-excited eigenvectors from each Onsager sector and to make the replacement $\varepsilon(\theta_j) \to -\varepsilon(\theta_j)$ for all excited θ_j in the final formula. We use the same formulas for the sector with charge Q and with parameters θ'_j, $j = 1, 2, \ldots, n$.

In each Onsager sector $\mathcal{V}^P$ we call the eigenvector of H with the lowest energy (that is without excitations) the *ground state* and denote it $|g.s.\rangle_P$. The matrix element between the ground states of two Onsager sectors with charges P and Q, $r = (Q - P) \bmod N$, is

$$_P\langle g.s.|Z_1^r|g.s.\rangle_Q = \sum_{V,V'} \prod_{i \in V} a_0(\theta_i) \prod_{i \in W} a_1(\theta_i) \prod_{i \in V'} a_0(\theta'_i) \prod_{i \in W'} a_1(\theta'_i) (S_{PQ})_{V,V'}.$$

The exact matrix elements $(S_{PQ})_{V,V'}$ are related to the matrix elements $(C_{PQ})_{V,V'}$ defined by (43), (39) by the relation (44). Then

$$_P\langle g.s.|Z_1^r|g.s.\rangle_Q$$

$$= \mathcal{N}_{PQ} \prod_{i=1}^m a_0(\theta_i) \prod_{i=1}^n a_1(\theta'_i) \sum_{V,V'} \prod_{i \in W} \left(-\frac{a_1(\theta_i)}{a_0(\theta_i)} \tan \frac{\theta_i}{2}\right) \prod_{i \in V'} \left(\frac{a_0(\theta'_i)}{a_1(\theta'_i)} \tan \frac{\theta'_i}{2}\right) K_I$$

$$= (-1)^n \mathcal{N}_{PQ}(2\mathsf{k}')^{\sigma(\mu-\alpha)/2 + \tau(\mu+\alpha)/2 + (\mu^2 - \alpha^2)/4} \prod_{i=1}^{\mu} \left(\frac{(\varepsilon_i + \varepsilon_0)(\varepsilon_\pi + \varepsilon_i)}{4\varepsilon_i}\right)^{1/2}$$

$$\times \sum_I \prod_{i \in \bar{I}} \left(\frac{\varepsilon_i - \varepsilon_0}{\varepsilon_\pi + \varepsilon_i}\right) \frac{\delta_{|I|,(\mu-\alpha)/2}}{\prod_{i \in I, j \in \bar{I}}(\varepsilon_j^2 - \varepsilon_i^2) \prod_{i \in I}(\varepsilon_\pi^2 - \varepsilon_i^2)^\sigma \prod_{i \in \bar{I}}(\varepsilon_0^2 - \varepsilon_i^2)^\tau}, \tag{58}$$

where we defined $\varepsilon_i = \varepsilon(\theta_i)$ for $1 \leq i \leq m$, $\varepsilon_i = -\varepsilon(\theta'_{i-m})$ for $m < i \leq m + n$ and $\varepsilon_0 = \varepsilon(0)$, $\varepsilon_\pi = \varepsilon(\pi)$. Also we used

$$\cos \theta - \cos \theta' = (\varepsilon^2(\theta') - \varepsilon^2(\theta))/(2\mathsf{k}'), \qquad \tan \frac{\theta}{2} = \sqrt{\frac{\varepsilon^2(\theta) - \varepsilon^2(0)}{\varepsilon^2(\pi) - \varepsilon^2(\theta)}},$$

$$-\tan \frac{\theta}{2} \cdot \frac{a_1(\theta)}{a_0(\theta)} = \frac{\varepsilon(\theta) - \varepsilon(0)}{\varepsilon(\pi) + \varepsilon(\theta)}, \qquad \tan \frac{\theta}{2} \cdot \frac{a_0(\theta)}{a_1(\theta)} = \frac{-\varepsilon(\theta) - \varepsilon(0)}{\varepsilon(\pi) - \varepsilon(\theta)}. \tag{59}$$

In order to perform the summation over I in (58) we have to discuss the cases of even and odd μ separately.

4.2 Summation in the Case of Even μ

In this case we have $\alpha = 0$, $\beta = \pm 1$. Let us consider the case $\beta = -1$. We have $\sigma = \tau = 0$.

We use the following summation formula:

$$\sum_I \frac{\delta_{|I|,\mu/2}}{\prod_{a \in I}(z_a + u) \prod_{b \in \bar{I}}(z_b + v) \prod_{a \in I, b \in \bar{I}}(z_a^2 - z_b^2)}$$
$$= \frac{(-1)^{\mu(\mu-2)/8}(u - v)^{\mu/2}}{\prod_c(z_c + u)(z_c + v) \prod_{c<s}(z_s + z_c)}, \tag{60}$$

which is proved in Appendix A. This formula at $z_i = \varepsilon_i$, $i = 1, \ldots, \mu$, and $u = -\varepsilon_0$, $v = \varepsilon_\pi$ gives

$$\sum_I \frac{\delta_{|I|,\mu/2}}{\prod_{i \in I}(\varepsilon_i - \varepsilon_0) \prod_{i \in \bar{I}}(\varepsilon_\pi + \varepsilon_i) \prod_{i \in I, j \in \bar{I}}(\varepsilon_j^2 - \varepsilon_i^2)}$$
$$= \frac{(-1)^{\mu(\mu-2)/8}(\varepsilon_\pi + \varepsilon_0)^{\mu/2}}{\prod_{i=1}^{\mu}(\varepsilon_i - \varepsilon_0)(\varepsilon_\pi + \varepsilon_i) \prod_{i<j}(\varepsilon_i + \varepsilon_j)}, \tag{61}$$

which we use to make the summation in (58):

$$_P\langle g.s.|Z_1^r|g.s.\rangle_Q$$
$$= \mathcal{N}_{PQ} \prod_{i=1}^m \sqrt{\frac{\varepsilon(\theta_i) + \varepsilon(0)}{2\varepsilon(\theta_i)(\varepsilon(\pi) + \varepsilon(\theta_i))}} \prod_{i=1}^n \sqrt{\frac{\varepsilon(\theta_i') - \varepsilon(0)}{2\varepsilon(\theta_i')(\varepsilon(\pi) - \varepsilon(\theta_i'))}}$$
$$\times \frac{(-1)^{(m+n)(m+n-2)/8+n(n+1)/2}(2k')^{(m+n)^2/4}}{\prod_{i<j}^m(\varepsilon(\theta_i) + \varepsilon(\theta_j)) \prod_{i<j}^n(\varepsilon(\theta_i') + \varepsilon(\theta_j')) \prod_{i=1}^m \prod_{j=1}^n(\varepsilon(\theta_i) - \varepsilon(\theta_j'))}. \tag{62}$$

Now let us consider the case of matrix elements between ground states of the ground state Onsager sectors for which $P < Q$ and $m = \mu/2$. In this case we can use the expression for $\mathcal{N}_{PQ}$ from (48) rewritten in terms of $\varepsilon(\theta)$

$$\mathcal{N}_{PQ} = (-1)^{mn}(2k')^{-mn} \prod_{j=1}^n \sqrt{\frac{\varepsilon^2(\pi) - \varepsilon^2(\theta_j')}{\varepsilon^2(\theta_j') - \varepsilon^2(0)}} \cdot \prod_{i=1}^m \prod_{j=1}^n (\varepsilon^2(\theta_i) - \varepsilon^2(\theta_j')) \tag{63}$$

(observe that $\mathcal{N}_{PQ}$ depends only on the squares of ε's) to get exact matrix elements of the spin operator between ground states

$$_P\langle g.s.|Z_1^r|g.s.\rangle_Q = \prod_{i=1}^m \sqrt{\frac{\varepsilon(\theta_i) + \varepsilon(0)}{2\varepsilon(\theta_i)(\varepsilon(\pi) + \varepsilon(\theta_i))}} \prod_{i=1}^m \sqrt{\frac{\varepsilon(\pi) + \varepsilon(\theta_i')}{2\varepsilon(\theta_i')(\varepsilon(\theta_i') + \varepsilon(0))}}$$
$$\times \frac{\prod_{i,j=1}^m(\varepsilon(\theta_i) + \varepsilon(\theta_j'))}{\prod_{i<j}^m(\varepsilon(\theta_i) + \varepsilon(\theta_j))(\varepsilon(\theta_i') + \varepsilon(\theta_j'))}. \tag{64}$$

In the case of general m, n and $\alpha = 0$, $\beta = 1$, $\sigma = \tau = 1$ the analogue of (62) is

$$_P\langle g.s.|Z_1^r|g.s.\rangle_Q = \mathcal{N}_{PQ} \prod_{i=1}^m \frac{1}{(\varepsilon(\pi) - \varepsilon(\theta_i))\sqrt{2\varepsilon(\theta_i)(\varepsilon(\theta_i) + \varepsilon(0))(\varepsilon(\pi) + \varepsilon(\theta_i))}}$$

$$\times \prod_{i=1}^n \frac{1}{(\varepsilon(\pi) + \varepsilon(\theta_i'))\sqrt{2\varepsilon(\theta_i')(\varepsilon(\theta_i') - \varepsilon(0))(\varepsilon(\pi) - \varepsilon(\theta_i'))}}$$

$$\times \frac{(-1)^{(m+n)(m+n-2)/8 + n(n+1)/2}(2k')^{m+n+(m+n)^2/4}}{\prod_{i<j}^m(\varepsilon(\theta_i) + \varepsilon(\theta_j)) \prod_{i<j}^n(\varepsilon(\theta_i') + \varepsilon(\theta_j')) \prod_{i=1}^m \prod_{j=1}^n (\varepsilon(\theta_i) - \varepsilon(\theta_j'))}.$$

$$(65)$$

This gives the matrix elements between ground states of the ground state Onsager sectors for which $P > Q$ and $m = \mu/2$ if one uses the corresponding $\mathcal{N}_{PQ}$ from (53). The final formula is analogous to (64) with additional factor $(-1)^m$ and with the replacement of the sets $\{\varepsilon(\theta_i)\} \leftrightarrow \{\varepsilon(\theta_j')\}$.

4.3 Summation in the Case of Odd μ

In the case of odd μ we have $\alpha = \pm 1$, $\beta = 0$. Let us consider the case $\alpha = -1$. Then $\sigma = 1$, $\tau = 0$.

In this case we will use another summation formula from Appendix A:

$$\sum_I \frac{\delta_{|I|,(\mu+1)/2}}{\prod_{a \in I}(z_a + u)(z_a + v) \prod_{a \in I, b \in \bar{I}}(z_a^2 - z_b^2)}$$

$$= \frac{(-1)^{(\mu+1)(\mu-1)/8}(u + v)^{(\mu-1)/2}}{\prod_c(z_c + u)(z_c + v) \prod_{c<s}(z_s + z_c)}.$$

It allows to perform the summation in (58) and get

$$_P\langle g.s.|Z_1^r|g.s.\rangle_Q = \frac{\mathcal{N}_{PQ}}{(\varepsilon(0) + \varepsilon(\pi))^{1/2}} \prod_{i=1}^m \frac{1}{\varepsilon(\pi) - \varepsilon(\theta_i)} \sqrt{\frac{\varepsilon(\theta_i) + \varepsilon(0)}{2\varepsilon(\theta_i)(\varepsilon(\pi) + \varepsilon(\theta_i))}}$$

$$\times \prod_{i=1}^n \frac{1}{\varepsilon(\pi) + \varepsilon(\theta_i')} \sqrt{\frac{\varepsilon(\theta_i') - \varepsilon(0)}{2\varepsilon(\theta_i')(\varepsilon(\pi) - \varepsilon(\theta_i'))}}$$

$$\times \frac{(-1)^{(\mu^2-1)/8 + n(n+1)/2}(2k')^{(\mu+1)^2/4}}{\prod_{i<j}^m(\varepsilon(\theta_i) + \varepsilon(\theta_j)) \prod_{i<j}^n(\varepsilon(\theta_i') + \varepsilon(\theta_j')) \prod_{i=1}^m \prod_{j=1}^n (\varepsilon(\theta_i) - \varepsilon(\theta_j'))}.$$

$$(66)$$

Now let us consider the case of matrix elements between ground states of the ground state Onsager sectors for which $P < Q$ and $m + 1$, $m = (\mu + 1)/2$, $n = (\mu - 1)/2$. In this case we can use the exact expression for $\mathcal{N}_{PQ}$ from (52) rewritten in terms of $\varepsilon(\theta)$:

$$\mathcal{N}_{PQ} = (-1)^{mn}(2\mathsf{k}')^{-mn}\prod_{i=1}^{m}\prod_{j=1}^{n}(\varepsilon^2(\theta_i) - \varepsilon^2(\theta_j'))\prod_{i=1}^{m}\frac{\varepsilon^2(\pi) - \varepsilon^2(\theta_i)}{2\mathsf{k}'}$$

$$\times \prod_{j=1}^{n}\sqrt{\frac{\varepsilon^2(\pi) - \varepsilon^2(\theta_j')}{\varepsilon^2(\theta_j') - \varepsilon^2(0)}}$$

to get the exact matrix elements between ground states:

$$_P\langle g.s.|Z_1^r|g.s.\rangle_Q = \prod_{i=1}^{m}\sqrt{\frac{(\varepsilon(\theta_i) + \varepsilon(0))(\varepsilon(\pi) + \varepsilon(\theta_i))}{2\varepsilon(\theta_i)}}$$

$$\times \prod_{i=1}^{n}\sqrt{\frac{1}{2\varepsilon(\theta_i')(\varepsilon(\theta_i') + \varepsilon(0))(\varepsilon(\pi) + \varepsilon(\theta_i'))}}$$

$$\times \frac{\prod_{i=1}^{m}\prod_{j=1}^{n}(\varepsilon(\theta_i) + \varepsilon(\theta_j'))}{(\varepsilon(\pi) + \varepsilon(0))^{1/2}\prod_{i<j}^{m}(\varepsilon(\theta_i) + \varepsilon(\theta_j))\prod_{i<j}^{n}(\varepsilon(\theta_i') + \varepsilon(\theta_j'))}. \tag{67}$$

In the case of general m, n and $\alpha = 1$, $\beta = 0$, $\sigma = 0$, $\tau = 1$ the analogue of (66) is

$$_P\langle g.s.|Z_1^r|g.s.\rangle_Q = \frac{\mathcal{N}_{PQ}}{(\varepsilon(0) + \varepsilon(\pi))^{1/2}}\prod_{i=1}^{m}\frac{1}{\sqrt{2\varepsilon(\theta_i)(\varepsilon(\theta_i) + \varepsilon(0))(\varepsilon(\pi) + \varepsilon(\theta_i))}}$$

$$\times \prod_{i=1}^{n}\frac{1}{\sqrt{2\varepsilon(\theta_i')(\varepsilon(\theta_i') - \varepsilon(0))(\varepsilon(\pi) - \varepsilon(\theta_i'))}}$$

$$\times \frac{(-1)^{(m+n+1)(m+n+3)/8+n(n+1)/2}(2\mathsf{k}')^{(m+n+1)^2/4}}{\prod_{i<j}^{m}(\varepsilon(\theta_i) + \varepsilon(\theta_j))\prod_{i<j}^{n}(\varepsilon(\theta_i') + \varepsilon(\theta_j'))\prod_{i=1}^{m}\prod_{j=1}^{n}(\varepsilon(\theta_i) - \varepsilon(\theta_j'))}. \tag{68}$$

It gives the matrix elements between ground states of the ground state Onsager sectors for which $P > Q$ and $m - 1$ if one uses the corresponding $\mathcal{N}_{PQ}$ from (54). The final formula is analogous to (67) with an additional factor $(-1)^n$ and with the replacement of the sets $\{\varepsilon(\theta_i)\} \leftrightarrow \{\varepsilon(\theta_j')\}$.

5 Order Parameters for the Superintegrable Chiral Potts Quantum Chain

5.1 Thermodynamic Limit of Ground State Matrix Elements

For the superintegrable chiral Potts quantum chain with Hamiltonian (1) we have $N - 1$ order parameters $\mathcal{S}_r$, $r = 1, 2, \ldots, N - 1$, which take non-zero values in the ferromagnetic phase $0 \le \mathsf{k}' < 1$ and are defined by the matrix elements between ground states of ground state Onsager sectors (labeled by charge P) in the thermodynamic limit:

$$\mathcal{S}_r = \lim_{L\to\infty} {}_P\langle g.s.|Z_1^r|g.s.\rangle_{P+r}. \tag{69}$$

At $0 \leq \mathsf{k}' < 1$ there is N-fold asymptotic ($L \to \infty$) degeneration of energies of these ground states. (In fact, for $\mathbb{Z}_3$ for $0.901\ldots < \mathsf{k}' < 1$ these translation invariant states are not the true ground states, i.e. states with lowest energies [27, 35, 37]. Due to level crossing, the lowest energy state becomes non-translationally invariant). In the paper [8], from perturbative calculations the formula for the order parameters

$$\mathcal{S}_r = (1 - \mathsf{k}'^2)^{r(N-r)/(2N^2)} \tag{70}$$

was conjectured. Recently this formula was proved by Baxter [10, 11] using functional relations and analytical properties. Below we derive this formula starting from the exact results for the matrix elements of spin operator between ground states in the chain of finite length L.

From (64) the square of ground states matrix elements in the case of m is

$$
{}_P\langle g.s.|Z_1^r|g.s.\rangle_{P+r}^2 = \frac{\prod_{i=1}^m (\varepsilon(\theta_i) + \varepsilon(0))(\varepsilon(\theta_i') + \varepsilon(\pi))}{\prod_{i=1}^m (\varepsilon(\theta_i) + \varepsilon(\pi))(\varepsilon(\theta_i') + \varepsilon(0))}
$$
$$
\times \frac{\prod_{i,j=1}^m (\varepsilon(\theta_i) + \varepsilon(\theta_j'))^2}{\prod_{i,j=1}^m (\varepsilon(\theta_i) + \varepsilon(\theta_j))(\varepsilon(\theta_i') + \varepsilon(\theta_j'))}, \tag{71}
$$

where the θ_i and θ_i' refer to the Onsager sectors with charges P and $P + r$, respectively.

In the case $m + 1$ from (67) the matrix element of the spin operator Z_1^r between the ground states is

$$
{}_P\langle g.s.|Z_1^r|g.s.\rangle_{P+r}^2 = \frac{\prod_{i=1}^m (\varepsilon(\theta_i) + \varepsilon(0))(\varepsilon(\theta_i) + \varepsilon(\pi))}{(\varepsilon(0) + \varepsilon(\pi)) \prod_{i=1}^n (\varepsilon(\theta_i') + \varepsilon(0))(\varepsilon(\theta_i') + \varepsilon(\pi))}
$$
$$
\times \frac{\prod_{i=1}^n \prod_{j=1}^m (\varepsilon(\theta_i') + \varepsilon(\theta_j))^2}{\prod_{i,j=1}^n (\varepsilon(\theta_i') + \varepsilon(\theta_j')) \prod_{i,j=1}^m (\varepsilon(\theta_i) + \varepsilon(\theta_j))}. \tag{72}
$$

From (69) and (70) the formula for the order parameters which we have to obtain in the thermodynamic limit is

$$\lim_{L \to \infty} {}_P\langle g.s.|Z_1^r|g.s.\rangle_{P+r}^2 = (1 - \mathsf{k}'^2)^{r(N-r)/N^2}. \tag{73}$$

First we consider the case of matrix elements of type (71) when m. Whereas up to now the θ_i and θ_i' were arbitrary, now we take them to be determined by the BAMP-polynomials of [5, 35]. We use the following relation for the thermodynamic limit:

$$\phi(\lambda) := \lim_{L \to \infty} \left(\sum_{i=1}^m \log(\lambda + \varepsilon(\theta_i)) - \sum_{i=1}^m \log(\lambda + \varepsilon(\theta_i')) \right) = \frac{r}{N} \log \frac{\lambda + 1 - \mathsf{k}'}{\lambda + 1 + \mathsf{k}'}, \tag{74}$$

where λ is an arbitrary parameter. The proof of this formula is given in Appendix B. The thermodynamic limit is taken in such a way as to keep the relation m and values of P and r. This limit can be realized by adding multiples of N to the chain length L.

Using (74) at $\lambda = \varepsilon(0) = 1 - \mathsf{k}'$ and $\lambda = \varepsilon(\pi) = 1 + \mathsf{k}'$ we obtain

$$\lim_{L \to \infty} \frac{\prod_{i=1}^m (\varepsilon(\theta_i) + \varepsilon(0))}{\prod_{i=1}^m (\varepsilon(\theta_i') + \varepsilon(0))} = (1 - \mathsf{k}')^{r/N}, \tag{75}$$

$$\lim_{L \to \infty} \frac{\prod_{i=1}^{m}(\varepsilon(\theta_i') + \varepsilon(\pi))}{\prod_{i=1}^{m}(\varepsilon(\theta_i) + \varepsilon(\pi))} = (1 + \mathsf{k}')^{r/N}. \tag{76}$$

The thermodynamic limit of the double products in (71) can be calculated along the following chain of equalities:

$$\lim_{L \to \infty} \log \frac{\prod_{i,j=1}^{m}(\varepsilon(\theta_i) + \varepsilon(\theta_j'))^2}{\prod_{i,j=1}^{m}(\varepsilon(\theta_i) + \varepsilon(\theta_j))(\varepsilon(\theta_i') + \varepsilon(\theta_j'))}$$

$$= \lim_{L \to \infty} \left(\sum_{i,j} \left(\log(\varepsilon(\theta_i) + \varepsilon(\theta_j')) - \log(\varepsilon(\theta_i') + \varepsilon(\theta_j')) \right) \right.$$

$$+ \sum_{i,j} \left(\log(\varepsilon(\theta_i') + \varepsilon(\theta_j)) - \log(\varepsilon(\theta_i) + \varepsilon(\theta_j)) \right) \Bigg)$$

$$= \lim_{L \to \infty} \sum_{j} \left(\phi(\varepsilon(\theta_j')) - \phi(\varepsilon(\theta_j)) \right)$$

$$= \lim_{L \to \infty} \frac{r}{N} \left(\sum_{j} \log(\varepsilon(\theta_j') + 1 - \mathsf{k}') - \sum_{j} \log(\varepsilon(\theta_j') + 1 + \mathsf{k}') \right.$$

$$\left. - \sum_{j} \log(\varepsilon(\theta_j) + 1 - \mathsf{k}') + \sum_{j} \log(\varepsilon(\theta_j) + 1 + \mathsf{k}') \right)$$

$$= \frac{r}{N}(-\phi(1 - \mathsf{k}') + \phi(1 + \mathsf{k}')) = -\frac{r^2}{N^2} \log(1 - \mathsf{k}'^2). \tag{77}$$

Exponentiating we get

$$\frac{\prod_{i,j=1}^{m}(\varepsilon(\theta_i) + \varepsilon(\theta_j'))^2}{\prod_{i,j=1}^{m}(\varepsilon(\theta_i) + \varepsilon(\theta_j))(\varepsilon(\theta_i') + \varepsilon(\theta_j'))} \to (1 - \mathsf{k}'^2)^{-r^2/N^2}. \tag{78}$$

Combining the latter relation with (75) and (76) we obtain (70).

In the case of the matrix elements (72) we have to use the same arguments but instead of the formula (74) we have to explore the relation

$$\lim_{L \to \infty} \left(\sum_{i=1}^{m} \log(\lambda + \varepsilon(\theta_i)) - \sum_{i=1}^{m-1} \log(\lambda + \varepsilon(\theta_i')) \right) = \frac{r}{N} \log \frac{\lambda + 1 - \mathsf{k}'}{\lambda + 1 + \mathsf{k}'} + \log(\lambda + 1 + \mathsf{k}'). \tag{79}$$

So, in both cases for the order parameter we obtain the famous result (73).

6 Conclusions

Starting from Baxter's extension of the Onsager algebra we have found factorized expressions for the spin operator matrix elements between the eigenstates of Hamiltonians of the finite length superintegrable $\mathbb{Z}_N$-symmetric chiral Potts quantum chain up to a scalar factor for any pair of the Onsager sectors.

Thus the problem of finding all the matrix elements is reduced to the calculation of these scalar factors. Derivation of these factors will probably require an information on the Bethe-states of τ_2-model and $sl(2)$-loop algebra symmetries. Further investigation in this direction is important since the knowledge of the explicit formulas for the matrix elements will be useful for the study of the correlation functions of the superintegrable chiral Potts chain (such correlation functions of the three state superintegrable chiral Potts spin chain of length 3, 4, 5 were studied in [38]). These scalar factors are known for the matrix elements between the ground states Onsager sectors and this allows to take the thermodynamics limit using the standard technique and to derive the order parameters of the superintegrable chiral Potts chain.

In the case $N = 2$ (the Ising quantum chain in a transverse field) these scalar factors can be found for all possible pairs of the Onsager sectors. This allows to obtain the factorized expression for the spin operator matrix elements in this model found in [16] in the framework of the method of Separation of Variables. We will address this problem in our forthcoming paper.

In the recent paper [15], Baxter has shown that the determinant representation (7.11) from [12] implies the factorized formulas for $(\mathcal{M}_r^{(2)})^2$, which in the thermodynamic limit give the order parameters of the SCPC. Baxter's formulas for $(\mathcal{M}_r^{(2)})^2$ coincide with our results (71) and (72). After submitting this paper, an alternative derivation of the spontaneous magnetization by Au-Yang and Perk appeared on the archive [41].

Appendix A: Proof of the Summation Formulas

In the case of even μ we have the following summation formula:

$$\sum_I \frac{\delta_{|I|,\mu/2}}{\prod_{a\in I}(z_a + u)\prod_{b\in \bar{I}}(z_b + v)\prod_{a\in I, b\in \bar{I}}(z_a^2 - z_b^2)}$$
$$= \frac{(-1)^{\mu(\mu-2)/8}(u - v)^{\mu/2}}{\prod_c(z_c + u)(z_c + v)\prod_{c<s}(z_s + z_c)}. \tag{80}$$

We start from the left-hand side. It does not have poles at $z_a = z_b$. Indeed, such a pole may arise when $a \in I$, $b \in \bar{I}$. But to each such summand there corresponds a summand with I replaced by $\tilde{I} = \{b\} \cup I \setminus \{a\}$. A straightforward analysis shows that the sum of these two summands does not contain a pole at $z_a = z_b$. Therefore the left-hand side can be presented as

$$\frac{P_\mu(u, v; z_1, z_2, \ldots, z_\mu)}{\prod_c(z_c + u)(z_c + v)\prod_{c<s}(z_s + z_c)},$$

where $P_\mu(u, v; z_1, z_2, \ldots, z_\mu)$ is a polynomial of the corresponding variables. Denote by d_c the degree of the rational function in the left hand side of (80) with respect to the variable z_c and estimate it. From the initial sum we have $d_c \leq -\mu - 1$. From the factorized expression

we have $d_c = \deg_{z_c} P_\mu - \mu - 1$. Hence $\deg_{z_c} P_\mu = 0$. That is P_μ does not depend on z_c for all c.

To find $P_\mu(u, v)$ let us analyze the pole at $z_1 \to -z_2$. Such pole arises if $1 \in I$, $2 \in \bar{I}$ or if $2 \in I$, $1 \in \bar{I}$. Then we separate factors depending on z_1 and z_2 and denote by I' and $\bar{I}'$ the sets I and $\bar{I}$ with 1 and 2 excluded. At $z_1 \to -z_2$ the summation is reduced to the summation over I' reducing the calculation of the sum to the same problem for $\mu - 2$. It gives the recurrent relation

$$P_\mu(u, v) = (-1)^{(\mu-2)/2}(u - v) P_{\mu-2}(u, v).$$

Calculating explicitly the sum at $\mu = 2$ we get $P_2(u, v) = (u - v)$. Therefore $P_\mu(u, v) = (-1)^{\mu(\mu-2)/8}(u - v)^{\mu/2}$. This proves the summation formula for even μ.

The summation formula for odd μ

$$\sum_I \frac{\delta_{|I|,(\mu+1)/2}}{\prod_{a \in I}(z_a + u)(z_a + v) \prod_{a \in I, b \in \bar{I}}(z_a^2 - z_b^2)}$$
$$= \frac{(-1)^{(\mu+1)(\mu-1)/8}(u + v)^{(\mu-1)/2}}{\prod_c (z_c + u)(z_c + v) \prod_{c < s}(z_s + z_c)}$$

can be proved in the same way.

Appendix B: Proof of (74)

The aim of this Appendix is to prove (74) and (79). The proof is close to the derivation presented in [39].

We use the BAMP polynomial in e^{Nu} of degree m

$$\Psi_P(u) = e^{-Pu} \sum_{k=0}^{N-1} \omega^{Pk} \left(\frac{1 - e^{Nu}}{1 - \omega^{-k}e^u} \right)^L. \tag{81}$$

In most papers the polynomial (81) is written in terms of the variable $z = e^u$ ([5], similarly in [35] etc.). The zeros of the polynomials Ψ_P are known to be all simple and to come on the negative real axis of the variable z^N. For the following, the use of the variable u will be useful: so, (81) has simple zeros at $u = u_1, u_2, \ldots, u_m$, where $u_1, u_2, \ldots, u_m$ can be chosen to have imaginary part π/N. Each zero e^{Nu_j} of this polynomial corresponds to a real value of θ_j, calculated through the relation
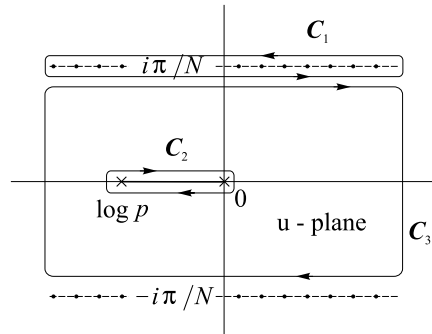
$$\cos\theta = (1 + e^{Nu})/(1 - e^{Nu}).$$

This relation also implies that $\operatorname{Re} u \to -\infty$ corresponds to $\theta = 0$, $\varepsilon(0) = 1 - \mathsf{k}'$, $\operatorname{Re} u \to +\infty$ corresponds to $\theta = \pi$, $\varepsilon(\pi) = 1 + \mathsf{k}'$.

We present the following sum as an integral along the contour C_1 shown in Fig. 1:

$$\sum_{i=1}^m \log(\lambda + \varepsilon(\theta_i)) = \oint_{C_1} \log\left(\frac{\varepsilon(\theta) + \lambda}{1 + \mathsf{k}' + \lambda} \right) \frac{\Psi_P'(u)}{\Psi_P(u)} \frac{du}{2\pi i}$$
$$+ \log(1 + \mathsf{k}' + \lambda) \oint_{C_1} \frac{\Psi_P'(u)}{\Psi_P(u)} \frac{du}{2\pi i}. \tag{82}$$

Fig. 1 Integration contours
C_1, C_2, C_3 used in Appendix B

The motivation for introducing the denominator $\log(1 + \mathsf{k}' + \lambda)$ in the first term of r.h.s of (82) will be given below. The integral in the second term gives m. The other sum entering (74), (79), and corresponding to sector with charge $P + r$, is given by a similar relation where the second term is $n \log(1 + \mathsf{k}' + \lambda)$. In the case of (74) we have m and the difference of these terms disappears. In the case of (79) we have $m + 1$ and the difference is $\log(1 + \mathsf{k}' + \lambda)$.

Let us analyze the first integral from the right-hand side of (82). Its integrand is analytic in the domain enclosed by contours C_1 and C_3 except for the simple poles enclosed by C_1 and a branch cut (where $\varepsilon(\theta)$ is pure imaginary) on the negative real axis along the segment $u \in [\log p, 0]$ (enclosed by C_2), where

$$\log p = \frac{2}{N} \log \frac{1 - \mathsf{k}'}{1 + \mathsf{k}'} < 0.$$

At $u \to 0$, $\varepsilon(\theta) \to \infty$. At $u \to \log p$, $\varepsilon(\theta) \to 0$.

The integral with the same integrand along the contour $C_1 - C_3$ gives 0. Indeed, the integral along the horizontal lines vanishes due to the periodicity of integrand under the transformation $u \to u + 2\pi \mathrm{i}/N$. The integral along the right vertical segment vanishes due to

$$\log \left(\frac{\varepsilon(\theta) + \lambda}{1 + \mathsf{k}' + \lambda} \right) \to 0.$$

This gives the motivation for introducing the denominator $1 + \mathsf{k}' + \lambda$ in the first integral in (82). The integral along the left vertical segment vanishes since $\Psi_P(u)$ is a polynomial in e^{Nu} with non-zero free term and therefore $\Psi_P'(u)/\Psi_P(u) \sim e^{Nu} \to 0$ as $\operatorname{Re} u \to -\infty$. Therefore instead of the integration along C_1 we may integrate along C_3.

Now we shrink the contour C_3 to C_2, that is around the branch cut. On C_2, the term in (81) with $k = 0$ exponentially dominates as $L \to \infty$. Indeed, the absolute value of the ratio of the term $k = 0$ and any other term $k \neq 0$ is the L-th power of

$$\frac{|1 - \omega^{-k} e^u|}{1 - e^u} > 1$$

with the left-hand side of the inequality minimized at $u = \log p$. Therefore in thermodynamic limit we can ignore the terms with $k \neq 0$ in the polynomial (81) and replace it by

$$e^{-Pu} [(1 - e^{Nu})/(1 - e^u)]^L$$

in the integral along C_2. Finally we expand the contour to C_3 and get

$$\frac{1}{2\pi i} \oint_{C_3} \log \left(\frac{\varepsilon(\theta) + \lambda}{1 + k' + \lambda} \right) \left(-P + L \left(-\frac{N}{1 - e^{-Nu}} + \frac{1}{1 - e^{-u}} \right) \right) du.$$

The terms proportional to L dominate at $L \to \infty$ but they do not depend on P and so they disappear in (74) and (79). Therefore the left-hand side of (74) in the limit $L \to \infty$ becomes

$$\frac{-P - (-(P + r))}{2\pi i} \oint_{C_3} \log \left(\frac{\varepsilon(\theta) + \lambda}{1 + k' + \lambda} \right) du$$

$$= \frac{r}{2\pi i} \log \left(\frac{1 - k' + \lambda}{1 + k' + \lambda} \right) \int_{-\infty - i\pi/N}^{-\infty + i\pi/N} du = \frac{r}{N} \log \left(\frac{1 - k' + \lambda}{1 + k' + \lambda} \right),$$

where we used the fact that the integral along the horizontal lines vanishes due to the period-icity of the integrand, and along the right vertical line due to vanishing the integrand. Only the left vertical line gives a constant contribution. Recall that $\mathrm{Re}\, u \to -\infty$ corresponds to $\theta = 0$, $\varepsilon(0) = 1 - k'$. In the case of (79) we have the same result but with the additional term $\log(1 + k' + \lambda)$ as was explained above.

Appendix C: Numerical Verification

Before starting our research we implemented a numerical verification of the finite-size for-mula (71), and compared this to the exact thermodynamic limit formula (70) for the order parameter. We approximate the angles θ_i and θ_i' for $L \to \infty$ as [40]

$$\cos \theta_l = \frac{\sin^N(K_l + \pi/N) - \sin^N(K_l)}{\sin^N(K_l + \pi/N) + \sin^N(K_l)},$$

$$K_l = \frac{2Nl + 2Q - N}{2NL} \pi, \ l = 1, 2, \ldots, m. \tag{83}$$

We fix $k' = 0.8$ and obtain:

$N = 3$, $L = 300$, $r = 1$:
Numerical calculation of (71) with (83): $|_{Q=1}\langle S \rangle_{Q=2}|^2 = 0.796894034089816$
Analytic formula: $(1 - k'^2)^{2/9} = 0.796893997784373$
Error: 3.63054×10^{-8}

$N = 5$, $L = 300$, $r = 1$:
Numerical calculation: $|_{Q=1}\langle S \rangle_{Q=2}|^2 = 0.8491969001045062$
Analytic formula: $(1 - k'^2)^{4/25} = 0.8491969000417509$
Error: 6.27554×10^{-11}

$N = 5$, $L = 300$, $r = 2$:
Numerical calculation: $|_{Q=1}\langle S \rangle_{Q=3}|^2 = 0.7825509089016481$
Analytic formula: $(1 - k'^2)^{6/25} = 0.7825509088837955$
Error: 1.07617×10^{-11}

These results of the numerical verification encouraged us to look for an analytical proof of (71).

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