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Form-factors in the Baxter–Bazhanov–Stroganov model II: Ising model on the finite lattice

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Abstract

We continue our investigation of the Baxter–Bazhanov–Stroganov or $\tau^{(2)}$-model using the method of separation of variables (von Gehlen *et al* 2006 *J. Phys. A: Math. Gen.* **39** 7257, 2007 *J. Phys. A: Math. Theor.* **40** 14117). In this paper we derive for the first time the factorized formula for form-factors of the Ising model on a finite lattice conjectured previously by Bugrij and Lisovyy (2003 *Phys. Lett.* A **319** 390, 2003 *J. Theor. Math. Phys.* **140** 987). We also find the matrix elements of the spin operator for the finite quantum Ising chain in a transverse field.

Dedicated to Professor Anatoly Bugrij on the occasion of his 60-th birthday

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1. Introduction

The Baxter–Bazhanov–Stroganov (BBS) model [5, 6] (also called the $\tau^{(2)}$-model, see e.g. [7, 8]) is associated with the cyclic L-operators [6, 9, 10] which act in a two-dimensional auxiliary space

$$L_j(\lambda) = \begin{pmatrix} 1 + \lambda\varkappa_j\mathbf{v}_j & \lambda\mathbf{u}_j^{-1}(a_j - b_j\mathbf{v}_j) \\ \mathbf{u}_j(c_j - d_j\mathbf{v}_j) & \lambda a_j c_j + \mathbf{v}_j b_j d_j/\varkappa_j \end{pmatrix}, \qquad (1)$$

where λ is the spectral parameter, and at each site $j = 1, \ldots, n$ we have five parameters a_j, b_j, c_j, d_j and $\varkappa_j$. At each site there is also an ultra-local Weyl algebra with elements $\mathbf{u}_j$ and $\mathbf{v}_j$ obeying

$$\mathbf{u}_j\mathbf{u}_k = \mathbf{u}_k\mathbf{u}_j, \qquad \mathbf{v}_j\mathbf{v}_k = \mathbf{v}_k\mathbf{v}_j, \qquad \mathbf{u}_j\mathbf{v}_k = \omega^{\delta_{j,k}}\mathbf{v}_k\mathbf{u}_j,$$
$$\omega = \mathrm{e}^{2\pi\mathrm{i}/N}, \qquad \mathbf{u}_k^N = \mathbf{v}_k^N = 1, \qquad N \in \mathbb{Z}_{\geqslant 2}.$$

Since ω is a root of unity, the Weyl operators can be represented naturally by matrices acting in the tensor product $\left(\mathbb{C}^N\right)^{\otimes n}$ [1, 2]. The monodromy matrix of the model is defined by

$$T_n(\lambda) = L_1(\lambda)L_2(\lambda)\cdots L_n(\lambda) = \begin{pmatrix} A_n(\lambda) & B_n(\lambda) \\ C_n(\lambda) & D_n(\lambda)\end{pmatrix}, \tag{2}$$

and the transfer matrix is its trace in the auxiliary space $\mathbf{t}_n(\lambda) = \operatorname{tr} T_n(\lambda)$ and gives rise to a set of commuting non-local and non-Hermitian Hamiltonians of the model:

$$\mathbf{t}_n(\lambda) = A_n(\lambda) + D_n(\lambda) = \mathbf{H}_0 + \mathbf{H}_1\lambda + \cdots + \mathbf{H}_{n-1}\lambda^{n-1} + \mathbf{H}_n\lambda^n.$$

Commutativity follows from the intertwining of $L_k(\lambda)$ by the asymmetric 6-vertex model R-matrix at root of unity.

In the present paper our focus will be on the case $N = 2$. As has been shown in [11], in this case the BBS model is related to a generalized Ising model with plaquette Boltzmann weights

$$W(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = a_0\left(1 + \sum_{1\leqslant i\leqslant j\leqslant 4} a_{ij}\sigma_i\sigma_j + a_4\sigma_1\sigma_2\sigma_3\sigma_4\right), \tag{3}$$

subject to the free-fermion condition $a_4 = a_{12}a_{34} - a_{13}a_{24} + a_{14}a_{23}$.

Generalizing Sklyanin's method of separation of variables (SoV) [12–14], in [1, 2] we have worked out a method to find common eigenvectors of the Hamiltonians $\mathbf{H}_m$. This proceeds in two steps[6]:

- Since $[B(\lambda), B(\mu)] = 0$, the off-diagonal element $B(\lambda)$ of the monodromy matrix (2) gives rise to an auxiliary set of commuting operators $\mathbf{h}_m$: $B(\lambda) = \mathbf{h}_1\lambda + \mathbf{h}_2\lambda^2 + \cdots + \mathbf{h}_n\lambda^n$. We construct their common right eigenvectors $|\Psi_\rho\rangle$ (the left eigenvectors $\langle\Psi_\rho|$ are obtained analogously) by an inductive procedure over the chain size n, starting from the one-site model. The eigenvalues of $B(\lambda)$ form a polynomial in λ of degree n, and from the intertwining relations we can show that

$$B(\lambda)|\Psi_\rho\rangle = \lambda r_0\omega^{-\rho_0}\prod_{k=1}^{n-1}(\lambda + r_k\omega^{-\rho_k})|\Psi_\rho\rangle, \qquad \boldsymbol{\rho} = (\rho_o, \rho_1, \ldots, \rho_{n-1}), \tag{4}$$

  where the amplitudes $(r_0, r_1, \ldots, r_{n-1})$ can be expressed in terms of the parameters of the model $a_j, \ldots, \varkappa_j$, and we can use the phases $\boldsymbol{\rho}$, $\rho_k \in \mathbb{Z}_N$, of the zeros

$$\nu_k = -r_k\omega^{-\rho_k}, \qquad k = 1, \ldots, n-1, \tag{5}$$

  of the eigenvalue polynomial for labelling the eigenvectors.
- Having solved the auxiliary problem, after a Fourier transformation of ρ_0 to ρ (ρ labels the $\mathbb{Z}_N$-charge sectors), the eigenvalue problem of $\mathbf{t}(\lambda) = A(\lambda) + D(\lambda)$ is reduced to the solution of Baxter equations. Using that $A(\nu_k)$ and $D(\nu_k)$ are raising and lowering operators on the auxiliary states $|\Psi_\rho\rangle$, we find that the periodic eigenstates $|\Phi_{\rho,\mathbf{E}}\rangle$ in

$$\mathbf{t}(\lambda)|\Phi_{\rho,\mathbf{E}}\rangle = t^{(\rho)}(\lambda|\mathbf{E})|\Phi_{\rho,\mathbf{E}}\rangle, \qquad \mathbf{E} = \{E_1, \ldots, E_{n-1}\}$$

[6] We consider a fixed chain length n, mostly suppressing the subscript n, which had been written explicitly in our previous papers, so $r_k \equiv r_{n,k}$ and $\rho_n \equiv \rho_{n,k}$ of [1, 2], etc.

with the eigenvalue polynomial $t^{(\rho)}(\lambda|\mathbf{E}) = E_0 + E_1\lambda + \cdots + E_n\lambda^n$ (where E_0 and E_n are directly known, see (20)) are obtained via the kernels $\mathcal{Q}^{\mathrm{R}}$ in

$$|\Phi_{\rho,\mathbf{E}}\rangle = \sum_{\rho_0,\boldsymbol{\rho}'} \omega^{-\rho\cdot\rho_0}\mathcal{Q}^{\mathrm{R}}(\boldsymbol{\rho}'|\rho,\mathbf{E})|\Psi_{\rho_0,\boldsymbol{\rho}'}\rangle, \qquad \boldsymbol{\rho}' = (\rho_1,\ldots,\rho_{n-1}). \quad (6)$$

The crucial fact is now (SoV) that after splitting off a known function $f(\boldsymbol{\rho}')$, the $n-1$-variable function $\mathcal{Q}^{\mathrm{R}}(\boldsymbol{\rho}'|\rho,\mathbf{E})$ factorizes into single-variable functions $Q_k^{\mathrm{R}}(\rho_k)$ (the ρ_k are the components of $\boldsymbol{\rho}'$, we often skip the charge index ρ of the Q_k^{R} etc):

$$\mathcal{Q}^{\mathrm{R}}(\boldsymbol{\rho}'|\rho,\mathbf{E}) = f(\boldsymbol{\rho}')\prod_{k=1}^{n-1} Q_k^{\mathrm{R}}(\rho_k),$$

and the $Q_k^{\mathrm{R}}(\rho_k)$ are determined by the Baxter equations ($k = 1,\ldots,n-1$):

$$t^{(\rho)}(v_k|\mathbf{E})Q_k^{\mathrm{R}}(\rho_k) = \Delta_k^+(v_k)Q_k^{\mathrm{R}}(\rho_k+1) + \Delta_k^-(\omega v_k)Q_k^{\mathrm{R}}(\rho_k-1). \quad (7)$$

The corresponding Baxter equations for the left periodic eigenvector read

$$t^{(\rho)}(v_k|\mathbf{E})Q_k^{\mathrm{L}}(\rho_k) = \omega^{n-1}\Delta_k^-(v_k)Q_k^{\mathrm{L}}(\rho_k+1) + \omega^{1-n}\Delta_k^+(\omega v_k)Q_k^{\mathrm{L}}(\rho_k-1). \quad (8)$$

The functions $\Delta_k^{\pm}$ are defined by

$$\Delta_k^+(\lambda) = (\omega^{\rho}/\chi_k)(\lambda/\omega)^{1-n}\prod_{m=1}^{n-1} F_m(\lambda/\omega), \qquad \Delta_k^-(\lambda) = \chi_k(\lambda/\omega)^{n-1}F_n(\lambda/\omega), \quad (9)$$

$$F_m(\lambda) = (b_m + \omega a_m \varkappa_m\lambda)\,(\lambda c_m + d_m/\varkappa_m)\,. \quad (10)$$

We shall not need the expression for χ_k, see (43) of [2], since this will cancel in our final formulae. The existence of a non-trivial solution to (7), (8) is provided by a set of functional equations, which determines the still unknown values $\mathbf{E}$.

In [2] we calculated the action of $\mathbf{u}_n$, the Weyl operator at site n, on an eigenvector $|\Psi_{\boldsymbol{\rho}}\rangle$ of $B(\lambda)$ to have the form

$$\mathbf{u}_n|\Psi_{\boldsymbol{\rho}}\rangle = g|\Psi_{\boldsymbol{\rho}}\rangle + \sum_{k=0}^{n-1} g_k|\Psi_{\boldsymbol{\rho}^{+k}}\rangle \qquad \text{with} \qquad \boldsymbol{\rho}^{+k} = (\rho_0,\ldots,\rho_k+1,\ldots,\rho_{n-1}), \quad (11)$$

and g and g_k are certain functions depending on the parameters $a_j, b_j, c_j, d_j, \varkappa_j$ and the components of $\boldsymbol{\rho}$. Since in [1, 2] we also found a factorized expression for the norm $\langle\Psi_{\boldsymbol{\rho}}|\Psi_{\boldsymbol{\rho}'}\rangle$, we have the framework for calculating normalized matrix elements $\langle\Psi_{\boldsymbol{\rho}}|\mathbf{u}_n|\Psi_{\boldsymbol{\rho}'}\rangle/\langle\Psi_{\mathbf{0}}|\Psi_{\mathbf{0}}\rangle$, where $\mathbf{0} = (0,0,\ldots,0)$. For calculating matrix elements between periodic states $\langle\Phi_{\rho}|\mathbf{u}_n|\Phi_{\rho'}\rangle$, in addition we also need the solutions $Q_k^{\mathrm{L,R}(\rho)}(\rho_k)$ of the Baxter equations (7) and (8) (recall that above we suppressed the charge index ρ). These are available for $N = 2$, and our main goal is to obtain such periodic matrix elements in a factorized form. We achieve this by explicitly performing the sums over the intermediate $\mathbb{Z}_2$-variables. For $N \geqslant 3$ the matrix element formula generalizing (58) of [2] can be written with no difficulties. However, since for $N \geqslant 3$ we have no explicit solutions to the Baxter equations, at present in this case we see no way to perform sums over intermediate variables.

This paper is organized as follows: in section 2 we recall the $N = 2$ spin matrix element calculated in [2] and transform it into a much more compact form by performing the summation over an intermediate variable, still keeping the model general and inhomogeneous. In order to proceed beyond this result, in section 3 we specialize the parameters of the BBS model such that we get the homogenous Ising model. We discuss the structure of the eigenvalues and the solutions to the Baxter equations. The vanishing of some transfer matrix eigenvalues at the zeros of $B(\lambda)$ requires us to distinguish four cases when solving the Baxter equations. Then in section 4 we continue the evaluation of the matrix elements of the spin operator, until we are finally able to perform the multiple sum over intermediate spins. The derivation of the basic formula for the multiple spin summation is delegated to the appendix. Section 5 deals with the calculation of squares of the matrix elements. In section 6 we include a special case excluded in the earlier sections and give the final formulae for the matrix element of spin operators in terms of the zeros of the transfer matrix and excited quasi-momenta. Then we are ready to compare our result in section 7 to a conjectured formula of Bugrij and Lisovyy [3, 4]. In section 8, we apply the formulae of section 6 to obtain the matrix element of σ^z for the finite quantum Ising chain in a transverse magnetic field. In section 9 we give our conclusions.

2. Spin operator matrix element for the $N = 2$ inhomogenous BBS model

In [2], we derived a formula for the normalized matrix element of the spin operator between arbitrary states of the periodic inhomogenous $N = 2$ BBS model. For $N = 2$ there are two $\mathbb{Z}_2$-charge sectors $\rho = 0, 1$ in (6). Since $\mathbf{u}_n$ is anticommuting with the charge operator $\mathbf{V} = \mathbf{v}_1\mathbf{v}_2\cdots\mathbf{v}_n$, its only non-vanishing matrix elements are between periodic states $|\Phi_\rho\rangle$ with different charge ρ. Let $Q^{\mathrm{L}(\rho)}$ and $Q^{\mathrm{R}(\rho)}$ be solutions to the Baxter equations (7), (8) and r_k the zeros of the operator polynomial $B(\lambda)$, see (4). Then our result in (58) of [2] can be written:

$$\frac{\langle\Phi_0|\mathbf{u}_n|\Phi_1\rangle}{\langle\tilde\Psi_{0,\mathbf{0}}|\tilde\Psi_{0,\mathbf{0}}\rangle} = \sum_{\rho'}\mathcal{N}(\boldsymbol{\rho}')\left(R_0(\boldsymbol{\rho}')\left(\frac{a_n}{\tilde r}(-1)^{\tilde\rho'} - \frac{\varkappa_1\varkappa_2\cdots\varkappa_{n-1}b_n}{r_0}\right) + \sum_{k=1}^{n-1}R_k(\boldsymbol{\rho}')\right), \tag{12}$$

$$\mathcal{N}(\boldsymbol{\rho}') = (-1)^{n\tilde\rho'}\prod_{l<m}^{n-1}\frac{r_l + r_m}{(-1)^{\rho_l}r_l + (-1)^{\rho_m}r_m}, \qquad R_0(\boldsymbol{\rho}') = \prod_{l=1}^{n-1}Q_l^{\mathrm{L}(0)}(\rho_l)Q_l^{\mathrm{R}(1)}(\rho_l), \tag{13}$$

$$R_k(\boldsymbol{\rho}') = -\frac{a_nb_nc_n}{r_0}Q_k^{\mathrm{L}(0)}(\rho_k+1)Q_k^{\mathrm{R}(1)}(\rho_k)\prod_{l\neq k}^{n-1}Q_l^{\mathrm{L}(0)}(\rho_l)Q_l^{\mathrm{R}(1)}(\rho_l) \times\left(1 - \frac{d_n}{\varkappa_nc_n\nu_k}\right)\frac{\nu_k^{n-1}\chi_k}{\prod_{s\neq k}(\nu_k-\nu_s)}, \tag{14}$$

with $\nu_k = -r_k(-1)^{\rho_k}, \tilde r = r_0r_1\cdots r_{n-1}$ and $\tilde\rho' = \sum_{k=1}^{n-1}\rho_k$. The different terms in (12) have the following origin: $\mathcal{N}(\boldsymbol{\rho}')$ is a normalization factor due to the convenient (since it avoids further factors) choice of normalizing by $\langle\tilde\Psi_{0,\mathbf{0}}|\tilde\Psi_{0,\mathbf{0}}\rangle$ of the auxiliary system. Here $|\tilde\Psi_{\rho,\rho'_n}\rangle = |\Psi_{0,\rho'_n}\rangle + (-1)^\rho|\Psi_{1,\rho'_n}\rangle$, where $|\Psi_{\rho_0,\rho'_n}\rangle$ is an eigenvector defined in (4), see also (35) in [2]. For the terms in (12) recall (11). The terms at $R_0(\boldsymbol{\rho}')$ correspond to g and g_0 in (11). The sum over k and the expression for $R_k(\boldsymbol{\rho}')$ arise from the shift in the index ρ_k and the coefficients g_k.

In the remaining part of this section we now show that the sum over k can be performed, leading to the much simpler expression (21) and (22).

We start rewriting the factors of the $R_k(\boldsymbol{\rho}')$:

$$-\frac{a_nb_nc_n}{r_0}\nu_k^{n-1}\chi_k\left(1-\frac{d_n}{\varkappa_nc_n\nu_k}\right) = \frac{(-1)^{n-1}b_n}{r_0\varkappa_n\nu_k(\nu_k+\zeta_n)}\Delta_k^{(0)-}(\nu_k)$$
$$= \frac{(-1)^{n-1}b_n}{r_0\varkappa_n\nu_k(\nu_k+\zeta_n)}\left\{\tfrac12\left(\Delta_k^{(0)+}(-\nu_k)+\Delta_k^{(0)-}(\nu_k)\right)+\tfrac12\left(\Delta_k^{(1)+}(-\nu_k)+\Delta_k^{(1)-}(\nu_k)\right)\right\}$$

$$= \frac{(-1)^{n-1}b_n}{2r_0\varkappa_n\nu_k(\nu_k+\zeta_n)}\left(\frac{(-1)^{n-1}t^{(0)}(\nu_k)Q_k^{\mathrm{L}(0)}(\rho_k)}{Q_k^{\mathrm{L}(0)}(\rho_k+1)}+\frac{t^{(1)}(-\nu_k)Q_k^{\mathrm{R}(1)}(\rho_k+1)}{Q_k^{\mathrm{R}(1)}(\rho_k)}\right), \tag{15}$$

where we define $\zeta_k = b_k/(a_k\varkappa_k)$ and use $\Delta_k^{(\rho)\pm}(\lambda)$ from (9), pointing out the explicit dependence on ρ. For obtaining the first two lines of (15) we used

$$\Delta_k^{(0)-}(\nu_k) = \Delta_k^{(1)-}(\nu_k) = \chi_k(-\nu_k)^{n-1}(b_n + a_n\varkappa_n\nu_k)(-\nu_k c_n + d_n/\varkappa_n),$$

and $\Delta_k^{(0)+}(-\nu_k) = -\Delta_k^{(1)+}(-\nu_k)$. To get the third line of (15) we used the Baxter equations (7), (8), where for $N = 2$ we have $\omega = -1$ and $\rho_k + 1 = \rho_k - 1 \bmod \mathbb{Z}_2$:

$$\frac{Q_k^{\mathrm{L}(0)}(\rho_k)}{Q_k^{\mathrm{L}(0)}(\rho_k+1)} = \frac{\Delta_k^{(0)+}(-\nu_k)+\Delta_k^{(0)-}(\nu_k)}{(-1)^{n-1}t^{(0)}(\nu_k)}, \qquad \frac{Q_k^{\mathrm{R}(1)}(\rho_k+1)}{Q_k^{\mathrm{R}(1)}(\rho_k)} = \frac{\Delta_k^{(1)+}(-\nu_k)+\Delta_k^{(1)-}(\nu_k)}{t^{(1)}(-\nu_k)}.$$

Then, using (15), (14) becomes

$$R_k(\boldsymbol{\rho}') = \frac{b_n}{2r_0\varkappa_n}\frac{1}{\nu_k(\nu_k+\zeta_n)\prod_{s\neq k}(\nu_k-\nu_s)}\Bigg(t^{(0)}(\nu_k)R_0(\boldsymbol{\rho}') + (-1)^{n-1}t^{(1)}(-\nu_k)$$
$$\times\, Q_k^{\mathrm{L}(0)}(\rho_k+1)Q_k^{\mathrm{R}(1)}(\rho_k+1)\prod_{l\neq k}^{n-1}Q_l^{\mathrm{L}(0)}(\rho_l)Q_l^{\mathrm{R}(1)}(\rho_l)\Bigg). \tag{16}$$

Now the sum over k in (12) can be performed using an identity (cf the appendix of [2]), valid for any polynomial $f(x)$ of degree less than $n+1$ and for any $n+1$ non-coincident points x_k: consider a polynomial $f(x) = f_n x^n + \cdots + f_0$, its interpolation through the points $x_1, \ldots, x_{n+1}$, and focussing attention on the coefficient of x^n:

$$f(x) = \sum_{k=1}^{n+1} f(x_k)\prod_{s\neq k}^{n+1}\frac{x-x_s}{x_k-x_s}, \qquad f_n = \sum_{k=1}^{n+1}\frac{f(x_k)}{\prod_{s\neq k}^{n+1}(x_k-x_s)}. \tag{17}$$

For calculating the sum over k of the first term in the parentheses of (16), in (17) we take $f(x) = t^{(0)}(x)$ and $(x_1, \ldots, x_{n-1}, x_n, x_{n+1}) = (\nu_1, \ldots, \nu_{n-1}, 0, -\zeta_n)$. Thus we get

$$\sum_{k=1}^{n-1}\frac{t^{(0)}(\nu_k)}{\nu_k(\nu_k+\zeta_n)\prod_{s\neq k}(\nu_k-\nu_s)} = E_n^{(0)} - \frac{t^{(0)}(0)}{\zeta_n\prod_{s=1}^{n-1}(-\nu_s)} - \frac{t^{(0)}(-\zeta_n)}{-\zeta_n\prod_{s=1}^{n-1}(-\zeta_n-\nu_s)}, \tag{18}$$

where $E_n^{(0)}$ is the leading coefficient of $t^{(0)}(\lambda)$.

For the second term of the last line of (16) we will not perform the summation over k directly. Instead, for each $\boldsymbol{\rho}'$ for which we make the summation of the first term, we take for the summation over k the second term of (16) corresponding to $\boldsymbol{\rho}'^{+k}$ (which entails $\nu_k \to -\nu_k$) in (12). Collecting all such terms and taking into account the changes which come from $\mathcal{N}(\boldsymbol{\rho}'^{+k})/\mathcal{N}(\boldsymbol{\rho}')$ we perform the summation over k. Together with (18), we get

$$\frac{b_n}{2r_0\varkappa_n}R_0(\boldsymbol{\rho}')\left(E_n^{(0)}-\frac{t^{(0)}(0)}{\zeta_n\prod_{s=1}^{n-1}(-\nu_s)}+\frac{t^{(0)}(-\zeta_n)}{\zeta_n\prod_{s=1}^{n-1}(-\zeta_n-\nu_s)}\right.$$
$$\left.-E_n^{(1)}-\frac{t^{(1)}(0)}{\zeta_n\prod_{s=1}^{n-1}(-\nu_s)}+\frac{t^{(1)}(\zeta_n)}{\zeta_n\prod_{s=1}^{n-1}(\zeta_n-\nu_s)}\right). \tag{19}$$

The leading and the constant coefficients of $t^{(\rho)}(\lambda)$ can be read off directly from (1), (2):

$$E_n^{(\rho)}=\prod_{l=1}^{n}a_lc_l+(-1)^\rho\prod_{l=1}^{n}\varkappa_l,\qquad E_0^{(\rho)}=t^{(\rho)}(0)=1+(-1)^\rho\prod_{l=1}^{n}(b_ld_l/\varkappa_l). \tag{20}$$

Inserting these results into (12) we find that the $E_n^{(\rho)}$ and $E_0^{(\rho)}$ terms in (19) just cancel the terms of the bracket at $R_0(\boldsymbol{\rho}')$ in (12), and we get simply

$$\frac{\langle\Phi_0|\mathbf{u}_n|\Phi_1\rangle}{\langle\tilde{\Psi}_{0,\mathbf{0}}|\tilde{\Psi}_{0,\mathbf{0}}\rangle}=\frac{a_n}{2r_0}\sum_{\boldsymbol{\rho}'\in\mathbb{Z}_2^{n-1}}\mathcal{N}(\boldsymbol{\rho}')R_0(\boldsymbol{\rho}')R(\boldsymbol{\rho}') \tag{21}$$

with

$$R(\boldsymbol{\rho}')=\frac{t^{(0)}(-\zeta_n)}{\prod_{l=1}^{n-1}(-\zeta_n+(-1)^{\rho_l}r_l)}+\frac{t^{(1)}(\zeta_n)}{\prod_{l=1}^{n-1}(\zeta_n+(-1)^{\rho_l}r_l)}. \tag{22}$$

We shall write $R(\boldsymbol{\rho}')=R^{(0)}(\boldsymbol{\rho}')+R^{(1)}(\boldsymbol{\rho}')$ when we have to refer to the separate terms on the right-hand side of (22). Despite the simple appearance, for the general inhomogenous $N=2$ BBS model, performing the multiple sums over the $\mathbb{Z}_2$ variables seems to be a presently impossible task. However, restricting ourselves to the homogenous model with the parameters satisfying

$$a_j=c_j=a,\qquad b_j=d_j=b,\qquad \varkappa_j=1\qquad \text{for}\quad j=1,\dots,n-1. \tag{23}$$

we are able to evaluate (21) with (13), (22) completely, as will be shown in section 4.

3. Homogeneous Ising model

In all the following sections we consider only the $N=2$ case of the model defined by (1) with (23). For a fixed chain length n, we are left with only the two parameters a, b and the spectral parameter λ. For $N=2$ we have $\omega=-1$ and represent the Weyl operators $\mathbf{u}_k$, $\mathbf{v}_k$ by Pauli matrices acting at the kth site. So, now our model is defined by

$$L_k(\lambda)=\begin{pmatrix}1+\lambda\sigma_k^x & \lambda\sigma_k^z(a-b\sigma_k^x)\\ \sigma_k^z(a-b\sigma_k^x) & \lambda a^2+\sigma_k^x b^2\end{pmatrix}. \tag{24}$$

Fixing the spectral parameter to the value $\lambda=b/a$, the L-operator (24) degenerates

$$L_k(b/a)=\left(1+\sigma_k^x b/a\right)\begin{pmatrix}1\\ a\sigma_k^z\end{pmatrix}\left(1,\quad b\sigma_k^z\right)$$

and the transfer matrix can be put into the standard Ising form

$$\mathbf{t}(b/a)=\operatorname{tr}L_1(b/a)L_2(b/a)\cdots L_n(b/a)=\prod_{k=1}^{n}\left(1+\sigma_k^x\cdot b/a\right)\cdot\prod_{k=1}^{n}\left(1+\sigma_{k-1}^z\sigma_k^z\cdot ab\right)$$
$$\sim\exp\left(\sum_{k=1}^{n}K_x^*\sigma_k^x\right)\exp\left(\sum_{k=1}^{n}K_x\sigma_{k-1}^z\sigma_k^z\right), \tag{25}$$

if we use periodic boundary conditions $\sigma^z_{n+k} \equiv \sigma^z_k$ and identify

$$e^{-2K_y} = \tanh K^*_x = b/a, \qquad \tanh K_x = ab. \tag{26}$$

So at $\lambda = b/a$ we call the model (24) the Ising model. If we do not fix the spectral parameter to this special value, we shall talk of the 'generalized Ising model'. However, transfer matrix eigenstates are independent of the choice of λ.

3.1. Structure of the eigenvalues

In [1] the eigenvalues of the transfer matrix $\mathbf{t}(\lambda) = \operatorname{tr} L_1(\lambda)\cdots L_n(\lambda)$ with $L_k(\lambda)$ given by (1) for $N = 2$ and homogeneous parameters have been calculated from the functional relations. From $\mathbb{Z}_2$-invariance $\mathbf{t}(\lambda)$ commutes with the $\mathbb{Z}_2$-charge operator $\mathbf{V} = \sigma^x_1\sigma^x_2\cdots\sigma^x_n$. Since $\mathbf{V}^2 = 1$, the space of eigenstates of $\mathbf{t}(\lambda)$ decomposes into two sectors according to the eigenvalues $(-1)^\rho$ (where $\rho = 0, 1$) of $\mathbf{V}$. The sector $\rho = 0$ is called the NS-sector, $\rho = 1$ the R-sector. The 2^n eigenvalues can be written as (we specialize assuming (23)):

$$t^{(\rho)}(\lambda) = (a^{2n} + (-1)^\rho)\prod_{\mathsf{q}}(\lambda + (-1)^{\sigma_{\mathsf{q}}} s_{\mathsf{q}}), \qquad s_{\mathsf{q}} = s_{-\mathsf{q}} = \sqrt{\frac{b^4 - 2b^2\cos\mathsf{q} + 1}{a^4 - 2a^2\cos\mathsf{q} + 1}}, \tag{27}$$

where the quasi-momentum q in each sector takes n values $\mathsf{q} = \frac{2\pi}{n}m$ with m integer (half-integer) for the R (NS)-sectors. If $\sigma_{\mathsf{q}} = 0$ the quasi-momentum q is called unexcited, for $\sigma_{\mathsf{q}} = 1$ it is called excited. In the NS (R)-sector, the eigenstates of $\mathbf{t}(\lambda)$ have an even (odd) number of excitations: $\prod_{\mathsf{q}}(-1)^{\sigma_{\mathsf{q}}} = (-1)^\rho$.

For $\mathsf{q} = 0$ (this occurs only for the R-sector) and for $\mathsf{q} = \pi$ we define

$$s_0 = \frac{b^2 - 1}{a^2 - 1}, \qquad s_\pi = \frac{b^2 + 1}{a^2 + 1}. \tag{28}$$

The quasi-momentum $\mathsf{q} = \pi$ is in the R-sector for n even, it is in the NS-sector for n odd. The different presence of factors $(\lambda \pm s_0)$ and $(\lambda \pm s_\pi)$ in (27) for n even or odd often makes it necessary to consider the cases of even n and odd n separately.

We shall also use the notation

$$\lambda_{\mathsf{q}} = (-1)^{\sigma_{\mathsf{q}}} s_{\mathsf{q}}. \tag{29}$$

3.2. State vectors from Baxter equations

In order to obtain the eigenvectors of the transfer matrix $\mathbf{t}(\lambda)$, we have to solve Baxter's equations (7) and (8). As input we use the corresponding eigenvalues $t^{(\rho)}(\lambda)$ which are specified by the values σ_{q} for all q in the sector ρ, see (27). Solving Baxter's equations, we should use the values $t^{(\rho)}(\pm r_k)$ of these polynomials at the values $\pm r_k$ of the roots of the eigenvalue polynomials of the operator $B_n(\lambda)$ (which is the off-diagonal element of the monodromy matrix) given by formula (A7) of [1]. For our special parameters (23) and $N = 2$ the r_k are simply related to the s_{q}:

$$r_k = s_{q_k}, \qquad q_k = \pi k/n, \qquad k = 1, \ldots, n-1. \tag{30}$$

This means that for our special choice of parameters (23), the zeros of $t^{(\rho)}(\lambda)$ may coincide with r_k, giving rise to the vanishing of the left-hand sides of (7) and (8). At the parameters (23) all F_m are equal: $F_m(\lambda) = F(\lambda)$ and from (10) we obtain

$$F(\lambda) = b^2 - a^2\lambda^2, \qquad \chi^2_k r^{2(n-1)}_k = (-1)^{n+k+1} F^{n-2}(r_k). \tag{31}$$

Let us compare two sets: the set $\{q_k\}$ which parameterizes the roots r_k, and the set of all possible quasi-momenta $\{\mathsf{q}\}$. The latter set is divided into two sub-sets: the NS and the R-sectors. The NS-sector contains pairs of quasi-momenta $\{q_k, -q_k\}$ for odd k and the R-sector includes the pairs $\{q_k, -q_k\}$ for even k. The quasi-momentum $\mathsf{q} = 0$ always belongs to the R-sector, and $\mathsf{q} = \pi$ belongs to the R-sector for even n and to the NS-sector for odd n.

The solutions of Baxter's equations for the case of the Ising model were found in [2]. Here we recall the final result. For a fixed sector ρ and the eigenvalue polynomial $t^{(\rho)}(\lambda)$ we have to solve $n-1$ systems of Baxter's equation (7) (or (8)) numerated by the integers $k = 1, \ldots, n-1$. With respect to these data we have to distinguish four cases. For $(-1)^\rho = (-1)^k$:

(i) $t^{(\rho)}(r_k) \neq 0$ and $t^{(\rho)}(-r_k) \neq 0$:

$$Q_k^{\mathrm{L,R}}(0) = 1, \qquad Q_k^{\mathrm{L,R}}(1) = \frac{(-1)^{n-1} t^{(\rho)}(-r_k)}{2\chi_k r_k^{n-1} F(r_k)}.$$

The other three cases occur for $(-1)^\rho = (-1)^{k-1}$:

(ii) $t^{(\rho)}(r_k) \neq 0$, $t^{(\rho)}(-r_k) = 0$: $t^{(\rho)}(\lambda)$ contains a factor $(\lambda + r_k)^2$ (both $\mathsf{q} = \pm q_k$ not excited), we may normalize

$$Q_k^{\mathrm{L,R}}(0) = 1, \qquad Q_k^{\mathrm{L,R}}(1) = 0.$$

(iii) $t^{(\rho)}(r_k) = 0$, $t^{(\rho)}(-r_k) \neq 0$: $t^{(\rho)}(\lambda)$ contains a factor $(\lambda - r_k)^2$ (both $\mathsf{q} = \pm q_k$ are excited), we cannot choose $Q_k^{\mathrm{L,R}}(0) = 1$, but we may normalize

$$Q_k^{\mathrm{L,R}}(0) = 0, \qquad Q_k^{\mathrm{L,R}}(1) = 1.$$

(iv) $t^{(\rho)}(r_k) = t^{(\rho)}(-r_k) = 0$: $t^{(\rho)}(\lambda)$ contains $\left(\lambda^2 - r_k^2\right)$ (either $\mathsf{q} = +q_k$ or $\mathsf{q} = -q_k$ is excited): a L'Hôpital procedure as described in [2] is required (in order to obtain eigenvectors of the translation operator) leading to

$$Q_k^{\mathrm{R}}(0) = Q_k^{\mathrm{L}}(0) = 1, \qquad Q_k^{\mathrm{R}}(1) = -Q_k^{\mathrm{L}}(1) = \frac{(-1)^{n+\sigma_{q_k}+1} 2\mathrm{i}\sin q_k t_{\check{q}_k}^{(\rho)}(-r_k)}{n\chi_k r_k^{n-1} A(q_k)},$$

where

$$t^{(\rho)}(\lambda) = t_{\check{q}_k}^{(\rho)}(\lambda)\left(\lambda + (-1)^{\sigma_{q_k}} s_{q_k}\right)\left(\lambda - (-1)^{\sigma_{q_k}} s_{-q_k}\right), \qquad A(\mathsf{q}) = a^4 - 2a^2\cos\mathsf{q} + 1. \quad (32)$$

In the following sections we shall restrict ourselves to calculate only transitions between eigenvectors allowing the normalization $Q_k^{\mathrm{L,R}}(0) = 1$, postponing to section 6 the consideration of eigenvectors for which $t^{(\rho)}(\lambda)$ contains factors $(\lambda - r_k)^2$, i.e. the eigenvectors involving case (iii) above.

As already observed at the beginning of section 2, the non-vanishing spin matrix elements have left and right eigenstates from different sectors. Let $t^{(0)}$ and $t^{(1)}$ be the corresponding eigenvalue polynomials. With respect to these two polynomials we define the sets $\check{\mathcal{D}}^{(\rho)}$, $\widehat{\mathcal{D}}^{(\rho)}$, $\mathcal{D}^{(\rho)}$:

$k \in \check{\mathcal{D}}^{(\rho)}$ if $t^{(\rho)}$ has a factor $(\lambda + r_k)^2$, i.e. we have case (ii),
$k \in \widehat{\mathcal{D}}^{(\rho)}$ if $t^{(\rho)}$ has a factor $(\lambda - r_k)^2$, case (iii),
$k \in \mathcal{D}^{(\rho)}$ if $t^{(\rho)}$ has a factor $\left(\lambda^2 - r_k^2\right)$, i.e. we have case (iv).

By $D = |\mathcal{D}|$ we denote the number of elements in $\mathcal{D} = \mathcal{D}^{(0)} \cup \mathcal{D}^{(1)}$, similarly for $\check{\mathcal{D}}$, etc.

4. Calculation of the matrix element of σ_n^z in the homogeneous Ising model

We now start to evaluate (21) with (13) and (22) in our simplified model where

$$\zeta = b/a, \qquad r_0^2 = (a^2 - b^2)(a^{4n} - 1)/(a^4 - 1). \tag{33}$$

We have to observe that in the derivation of (12) given in [2], generic BBS parameters leading to $t^{(\rho)}(r_k) \neq 0$ were assumed, and the solutions to the Baxter equation were normalized to $Q_k^{\mathrm{L,R}}(0) = 1$. As we have seen in section 3.2, in the case (iii) this normalization is not possible for the special parameters (23). In order not to complicate the derivation, in the following part of this section we shall simply exclude state vectors containing $k \in \widehat{\mathcal{D}}$, adding the changes necessary for $k \in \widehat{\mathcal{D}}$ in section 6. Also in this section we shall omit the superscripts L and R in the notations of $Q_k^{\mathrm{L,R}(\rho)}(\rho_k)$ supposing that the left/right eigenvectors are from NS/R-sectors as they appear in (21).

Consider $R_0(\boldsymbol{\rho}')$. Always one of the factors in $Q_l^{(0)}(\rho_l)Q_l^{(1)}(\rho_l)$ is from case (i) above, and excluding $l \in \widehat{\mathcal{D}}$, the other is from either (ii) or (iv). So always $Q_l^{(0)}(0)Q_l^{(1)}(0) = 1$. For $l \in \check{\mathcal{D}}$ we have $Q_l^{(0)}(1)Q_l^{(1)}(1) = 0$ since either $Q_l^{(0)}(1) = 0$ or $Q_l^{(1)}(1) = 0$ depending on the parity of l. So, in (21) the summation reduces to the summation over ρ_l for $l \in \mathcal{D}$, with $\rho_l = 0$ fixed for $l \in \check{\mathcal{D}}$.

4.1. Calculation of $R(\boldsymbol{\rho}')$

Let us show that a common factor can be extracted from the two terms of (22). We first consider the case of odd n where $\mathsf{q} = 0$ appears in the R-sector and $\mathsf{q} = \pi$ in the NS-sector.

We start with the first term $R^{(0)}(\boldsymbol{\rho}')$ in (22). Now from (27) the NS eigenvalue polynomial $t^{(0)}(\lambda)$ for odd n is

$$\text{NS, } n \text{ odd:} \qquad t^{(0)}(\lambda) = (a^{2n}+1)\big(\lambda + (-1)^{\sigma_\pi} s_\pi\big) \prod_{k\in\check{\mathcal{D}}^{(0)}} (\lambda + r_k)^2 \prod_{l\in\mathcal{D}^{(0)}} \big(\lambda^2 - r_l^2\big) \tag{34}$$

(for even n omit the bracket with s_π) since in the NS-sector only odd k appear, and these fall into one of the classes (ii) and (iv), class (iii) being momentarily excluded. We insert $t^{(0)}(-\zeta)$ from (34) and decompose the denominator product over l in its even-l and odd-l parts. We write the odd part as $l \in \mathcal{D}^{(0)} \cup \check{\mathcal{D}}^{(0)}$ since for $\rho = 0$ in cases (ii) and (iv) l must be odd (recall, we still exclude case (iii)):

$$R^{(0)}(\boldsymbol{\rho}') = (a^{2n}+1)\frac{\big(-\zeta + (-1)^{\sigma_\pi} s_\pi\big)}{\prod_{l\,\text{even}}\big(-\zeta + (-1)^{\rho_l} r_l\big)} \frac{\prod_{k\in\check{\mathcal{D}}^{(0)}}(-\zeta + r_k)^2 \prod_{l\in\mathcal{D}^{(0)}}\big(\zeta^2 - r_l^2\big)}{\prod_{k\in\check{\mathcal{D}}^{(0)}}(-\zeta + r_k)\prod_{l\in\mathcal{D}^{(0)}}\big(-\zeta + (-1)^{\rho_l} r_l\big)}$$
$$\times \frac{\prod_{m\in\check{\mathcal{D}}^{(1)}}(\zeta + r_m)\prod_{m\in\mathcal{D}^{(1)}}\big(\zeta + (-1)^{\rho_m} r_m\big)}{\prod_{m\,\text{even}}\big(\zeta + (-1)^{\rho_m} r_m\big)}. \tag{35}$$

In the last line we put a factor unity, written as quotient of upstairs a product over $m \in \mathcal{D}^{(1)} \cup \check{\mathcal{D}}^{(1)}$ and downstairs over m even. In the $\check{\mathcal{D}}$ terms we omitted the factor $(-1)^{\rho_k}$ since from (ii) this contributes only if $\rho_k = 0$. Now several cancellations take place, resulting in

$$R^{(0)}(\boldsymbol{\rho}') = \frac{(a^{2n}+1)\big(-\zeta + (-1)^{\sigma_\pi} s_\pi\big)}{(-1)^{|\mathcal{D}^{(0)}|}\prod_{l\,\text{even}}\big(-\zeta^2 + r_l^2\big)} \prod_{k\in\check{\mathcal{D}}}((-1)^k\zeta + r_k) \prod_{l\in\mathcal{D}}(\zeta + (-1)^{\rho_l} r_l). \tag{36}$$

Observe that now the $\boldsymbol{\rho}'$-dependence appears only in the last product over $\mathcal{D}$. This happens because all l-odd terms cancel and because $\check{\mathcal{D}}^{(0)}$ allows only $\rho_l = 0$. In the denominator we use $\zeta = b/a$, (27), (30) and $\prod_{l\text{ even}} A(q_l) = (a^{2n}-1)/(a^2-1)$ to obtain

$$\prod_{l\text{ even}} \left(-\zeta^2 + r_l^2\right) = ((\zeta^2-1)(a^2b^2-1))^{(n-1)/2}(a^2-1)/(a^{2n}-1). \tag{37}$$

The second term in (22) can be evaluated analogously. We insert $t^{(1)}(\zeta)$ from

$$\text{R, } n \text{ odd:} \qquad t^{(1)}(\lambda) = (a^{2n}-1)\left(\lambda + (-1)^{\sigma_0}s_0\right)\prod_{k\in\check{\mathcal{D}}^{(1)}}(\lambda+r_k)^2 \prod_{l\in\mathcal{D}^{(1)}}\left(\lambda^2 - r_l^2\right) \tag{38}$$

and use $\prod_{l\text{ odd}} A(q_l) = (a^{2n}+1)/(a^2+1)$ to get finally for n odd:

$$R^{(n\text{ odd})}(\boldsymbol{\rho}') = \Bigg((-1)^{\sigma_\pi}(a^2+1)\left(-\zeta + (-1)^{\sigma_\pi}s_\pi\right)\prod_{l\in\mathcal{D}}((-1)^{\rho_l}r_l+\zeta)$$
$$- (-1)^{\sigma_0}(a^2-1)\left(\zeta + (-1)^{\sigma_0}s_0\right)\prod_{l\in\mathcal{D}}((-1)^{\rho_l}r_l-\zeta)\Bigg)\mathsf{R} \tag{39}$$

with (using also (33))

$$\mathsf{R} = r_0^2\boldsymbol{\alpha}^{-1}(\boldsymbol{\alpha}\boldsymbol{\beta})^{-(n-1)/2}a^{n-1}\prod_{k\in\check{\mathcal{D}}}((-1)^k\zeta + r_k), \tag{40}$$

where $\boldsymbol{\alpha} = a^2 - b^2$, $\boldsymbol{\beta} = 1 - a^2b^2$, and $(-1)^{|\mathcal{D}^{(0)}|} = (-1)^{\sigma_\pi}$, $(-1)^{|\mathcal{D}^{(1)}|} = -(-1)^{\sigma_0}$ in the case of odd n.

The case of n even is less symmetric between $R^{(0)}$ and $R^{(1)}$ since now both $\mathsf{q} = 0$ and $\mathsf{q} = \pi$ are in the R-sector, none of them in NS. So the term containing s_π appears in $t^{(1)}(\zeta)$ instead of $t^{(0)}(-\zeta)$. Also, $(-1)^{|\mathcal{D}^{(0)}|} = 1$, $(-1)^{|\mathcal{D}^{(1)}|} = -(-1)^{\sigma_0+\sigma_\pi}$ in the case of even n. In the following products, for l odd there are $n/2$ values and for l even we have $n/2-1$ values:

$$R^{(n\text{ even})}(\boldsymbol{\rho}') = \Bigg(\prod_{l\in\mathcal{D}}((-1)^{\rho_l}r_l+\zeta) - (-1)^{\sigma_0+\sigma_\pi}\prod_{l\in\mathcal{D}}((-1)^{\rho_l}r_l-\zeta)$$
$$\times (a^4-1)\left(\zeta+(-1)^{\sigma_0}s_0\right)\left(\zeta+(-1)^{\sigma_\pi}s_\pi\right)a^2/(\boldsymbol{\alpha}\boldsymbol{\beta})\Bigg)\mathsf{R}, \tag{41}$$

$$\mathsf{R} = r_0^2\boldsymbol{\alpha}^{-1}(\boldsymbol{\alpha}\boldsymbol{\beta})^{1-n/2}a^{n-2}\prod_{k\in\check{\mathcal{D}}}((-1)^k\zeta + r_k). \tag{42}$$

4.2. *Calculation of $\mathcal{N}(\boldsymbol{\rho})\cdot R_0(\boldsymbol{\rho}')$*

In this subsection we shall show that the product $\mathcal{N}(\boldsymbol{\rho})\cdot R_0(\boldsymbol{\rho}')$ can be put into the very simple form (50). Let us start evaluating $R_0(\boldsymbol{\rho}')$.

At the beginning of this section we already discussed that, if we exclude case (iii), $l \neq \widehat{\mathcal{D}}$, then $Q_l^{(0)}(0)Q_l^{(1)}(0) = 1$, and from (ii) if $l\in\check{\mathcal{D}}$ we have $Q_l^{(0)}(1)Q_l^{(1)}(1) = 0$. So we have to consider only $l\in\mathcal{D}$ for which we get from (i) and (iv) (momentarily we suppose that l is odd, but the result (46) is the same for even l):

$$Q_l^{(0)}(1)Q_l^{(1)}(1) = -(-1)^{\sigma_{q_l}+l}\frac{(-1)^n 2\mathrm{i}\sin q_l t_{\check{q}_l}^{(0)}(-r_l)}{n\chi_l r_l^{n-1}A(q_l)}\cdot\frac{(-1)^{n-1}t^{(1)}(-r_l)}{2\chi_l r_l^{n-1}F(r_l)}$$
$$= (-1)^{\sigma_{q_l}+n+1}\frac{\mathrm{i}\sin q_l}{nA(q_l)F^{n-1}(r_l)}t_{\check{q}_l}^{(0)}(-r_l)t^{(1)}(-r_l), \tag{43}$$

where in the last step we used (31). The polynomial $t^{(0)}_{\breve{q}_l}(\lambda)$ is $t^{(0)}(\lambda)$ given by (34) with the factor $\lambda^2 - r_l^2$ omitted, see (32). In the first line the factor $-(-1)^{\sigma_{q_l}+l}$ takes care whether q_l or $-q_l$ is excited, the minus sign comes because $Q_l^{(0)}$ is a left eigenvector component. Now since we should not use $l \in \breve{\mathcal{D}}$ (if present, such a term leads to a vanishing contribution in (21)), we have

$$\begin{aligned} t^{(0)}_{\breve{q}_l}(-r_l)t^{(1)}(-r_l) &= \frac{a^{4n}-1}{a^4-1} S_l \prod_{m\in\mathcal{D},m\neq l} \left(r_l^2 - r_m^2\right) \\ &= \frac{a^{4n}-1}{a^4-1} S_l \prod_{k=1,k\neq l}^{n-1} \left(r_l^2 - r_k^2\right) \prod_{k\in\breve{\mathcal{D}}} \left(-\frac{-r_l+r_k}{r_l+r_k}\right) \end{aligned} \tag{44}$$

with $S_l := (a^4-1)\big(-r_l + (-1)^{\sigma_\pi} s_\pi\big)\big(-r_l + (-1)^{\sigma_0} s_0\big)$. Inserting (44) into (43) and using, recall (32),

$$r_l^2 - r_k^2 = 2(\cos q_k - \cos q_l)F(r_l)/A(q_k), \qquad \prod_{k=1}^{n-1} A(q_k) = \frac{a^{4n}-1}{a^4-1} = \frac{r_0^2}{a^2-b^2}, \tag{45}$$

and the trigonometric identity

$$2^{n-1}\sin^2 q_l \prod_{k\neq l} (\cos q_l - \cos q_k) = n(-1)^{l+1}$$

we obtain

$$Q_l^{(0)}(1)Q_l^{(1)}(1) = (-1)^{\sigma_{q_l}+l+|\breve{\mathcal{D}}|+1} \frac{S_l}{2\mathrm{i}\sin q_l F(r_l)} \prod_{k\in\breve{\mathcal{D}}} \left(\frac{-r_l+r_k}{r_l+r_k}\right), \tag{46}$$

valid both for q_l in R and for q_l in NS.

Let us rewrite the ratio $S_l/(2\mathrm{i}\sin q_l F(r_l))$ in a convenient way. By the straightforward use of definitions (28), (31) and (30) we find

$$\begin{aligned} &\mp\frac{S_l}{2\mathrm{i}\sin q_l F(r_l)} = \frac{-r_l + (-1)^{\sigma_0}\alpha_{\pm q_l}}{r_l + (-1)^{\sigma_0}\alpha_{\pm q_l}}, \qquad \alpha_q = \frac{b^2 - \mathrm{e}^{\mathrm{i}q}}{a^2 - \mathrm{e}^{\mathrm{i}q}} \qquad \text{for} \quad (-1)^{\sigma_0} = +(-1)^{\sigma_\pi}, \\ &\mp\frac{S_l}{2\mathrm{i}\sin q_l F(r_l)} = \frac{-r_l + (-1)^{\sigma_0}\beta_{\pm q_l}}{r_l + (-1)^{\sigma_0}\beta_{\pm q_l}}, \qquad \beta_q = \frac{b^2\mathrm{e}^{\mathrm{i}q} - 1}{a^2 - \mathrm{e}^{\mathrm{i}q}} \qquad \text{for} \quad (-1)^{\sigma_0} = -(-1)^{\sigma_\pi}, \end{aligned} \tag{47}$$

leading to (written such that it is valid for both $\rho_l = 0$ and $\rho_l = 1$):

$$Q_l^{(0)}(\rho_l)Q_l^{(1)}(\rho_l) = (-1)^{(n-1)\rho_l} \frac{(-1)^{\rho_l} r_l + \xi_l}{r_l + \xi_l} \cdot \prod_{k\in\breve{\mathcal{D}}} \frac{(-1)^{\rho_l} r_l + r_k}{r_l + r_k}, \tag{48}$$

where

$$\xi_l = \begin{cases} \tilde{\alpha}_l = (-1)^{\sigma_0}\alpha_{\tilde{q}_l} \\ \tilde{\beta}_l = (-1)^{\sigma_0}\beta_{\tilde{q}_l} \end{cases} \quad \text{for} \quad (-1)^{\sigma_0} = \pm(-1)^{\sigma_\pi}; \qquad \tilde{q}_l = (-1)^{\sigma_{q_l}+|\mathcal{D}|+l} q_l. \tag{49}$$

Multiplying by $\mathcal{N}(\boldsymbol{\rho}')$, it is easy to see that the products over $k \in \breve{\mathcal{D}}$ in (48) cancel (recall that $\rho_k = 0$ for $k \in \breve{\mathcal{D}}$) and we get finally

$$\mathcal{N}(\boldsymbol{\rho}) \cdot R_0(\boldsymbol{\rho}') = \prod_{l\in\mathcal{D}} (-1)^{\rho_l} \frac{(-1)^{\rho_l} r_l + \xi_l}{r_l + \xi_l} \prod_{m\in\mathcal{D},m>l} \frac{r_l + r_m}{(-1)^{\rho_l} r_l + (-1)^{\rho_m} r_m}. \tag{50}$$

4.3. Summation over $\boldsymbol{\rho}'$ in (21)

In (39), (41) and (50) we have obtained all factors for the calculation of the normalized matrix element in such a form that the dependence on the summation indices $\boldsymbol{\rho}'$ is explicit

$$\frac{\langle\Phi_0|\sigma_n^z|\Phi_1\rangle}{\langle\tilde{\Psi}_{\mathbf{0}}|\tilde{\Psi}_{\mathbf{0}}\rangle} = \sum_{\boldsymbol{\rho}'\in\mathbb{Z}_2^{n-1}} \left(\mathcal{R}_+^\nu \prod_{l\in\mathcal{D}}((-1)^{\rho_l}r_l+\zeta) + \mathcal{R}_-^\nu \prod_{l\in\mathcal{D}}((-1)^{\rho_l}r_l-\zeta)\right) \times \prod_{l\in\mathcal{D}}(-1)^{\rho_l}\frac{(-1)^{\rho_l}r_l+\xi_l}{r_l+\xi_l}\prod_{m\in\mathcal{D},m>l}\frac{r_l+r_m}{(-1)^{\rho_l}r_l+(-1)^{\rho_m}r_m}, \tag{51}$$

where the $\boldsymbol{\rho}'$-independent factors $\mathcal{R}_\pm^\nu$ can be read off from (39), (40) and (41), (42). The superscript ν stands for n odd and even, respectively.

Collecting all factors which depend on ρ_l, $l\in\mathcal{D}$, the problem of performing the multiple summation over ρ_l, $l\in\mathcal{D}$, reduces to calculating the following sum (proved in the appendix):

$$Y_\mathcal{D} = \sum_{\rho_l,l\in\mathcal{D}} \frac{\prod_{l\in\mathcal{D}}(-1)^{\rho_l}((-1)^{\rho_l}r_l+\xi_l)((-1)^{\rho_l}r_l+\zeta)}{\prod_{l<m,l,m\in\mathcal{D}}((-1)^{\rho_l}r_l+(-1)^{\rho_m}r_m)}$$
$$= \begin{cases} c_\alpha(b\pm a)\big(\prod_{j\in\mathcal{D}}\mathrm{e}^{\mathrm{i}\tilde{q}_j}\mp ab\big)\dfrac{\prod_{l\in\mathcal{D}}(2r_l/a)f_l^{(D-1)/2}g_l^{(D-3)/2}}{\prod_{l,m\in\mathcal{D},l<m}(\pm h_{l,m})}, & \xi_l=\pm\alpha_{\tilde{q}_l},\quad D \text{ odd} \\ c_\beta(1\mp ab)\big(\pm ab\prod_{j\in\mathcal{D}}\mathrm{e}^{\mathrm{i}\tilde{q}_j}+1\big)\dfrac{\prod_{l\in\mathcal{D}}(2r_l/a)(f_lg_l)^{D/2-1}}{\prod_{l,m\in\mathcal{D},l<m}(\pm h_{l,m})}, & \xi_l=\pm\beta_{\tilde{q}_l},\quad D \text{ even} \end{cases} \tag{52}$$

with $D=|\mathcal{D}|$,

$$c_\alpha=\boldsymbol{\alpha}^{-(D-1)(D-3)/4}(-\boldsymbol{\beta})^{-(D-1)^2/4},\qquad c_\beta=(-\boldsymbol{\alpha})^{-(D-2)D/4}\boldsymbol{\beta}^{-(D-2)^2/4}, \tag{53}$$

and we abbreviate

$$f_l=a^2\mathrm{e}^{\mathrm{i}\tilde{q}_l}-1,\qquad g_l=\mathrm{e}^{\mathrm{i}\tilde{q}_l}-a^2,\qquad h_{l,m}=\mathrm{e}^{\mathrm{i}\tilde{q}_l+\mathrm{i}\tilde{q}_m}-1,$$
$$\boldsymbol{\alpha}=a^2-b^2,\qquad \boldsymbol{\beta}=1-a^2b^2. \tag{54}$$

In the calculation of the matrix element (21), we restrict ourselves to the case $\sigma_0=\sigma_\pi$ corresponding to D odd. The case $\sigma_0\neq\sigma_\pi$ corresponding to D even can be done similarly. Also the two cases of even and odd parity of n have to be considered separately. For odd n, taking into account (39), (52) and using (28) with

$$(-1)^{\sigma_0}a(a^2+1)\big(-\zeta+(-1)^{\sigma_0}s_\pi\big)((-1)^{\sigma_0}a+b)\left(\prod_{l\in\mathcal{D}}\mathrm{e}^{\mathrm{i}\tilde{q}_l}-(-1)^{\sigma_0}ab\right)$$
$$-(-1)^{\sigma_0}a(a^2-1)\big(\zeta+(-1)^{\sigma_0}s_0\big)((-1)^{\sigma_0}a-b)\left(\prod_{l\in\mathcal{D}}\mathrm{e}^{\mathrm{i}\tilde{q}_l}+(-1)^{\sigma_0}ab\right)$$
$$=2(-1)^{\sigma_0}\boldsymbol{\alpha}(1-(-1)^{\sigma_0}ab)\prod_{l\in\mathcal{D}}\mathrm{e}^{\mathrm{i}\tilde{q}_l}, \tag{55}$$

we have finally

$$\frac{\langle\Phi_0|\sigma_n^z|\Phi_1\rangle}{\langle\tilde{\Psi}_{0,\mathbf{0}}|\tilde{\Psi}_{0,\mathbf{0}}\rangle} = r_0\tilde{c}_nc_\alpha\prod_{k\in\check{\mathcal{D}}}((-1)^kb+ar_k)\frac{\prod_{l\in\mathcal{D}}2r_l\,\mathrm{e}^{\mathrm{i}\tilde{q}_l}f_l^{(D-1)/2}g_l^{(D-3)/2}}{\prod_{l<m,l,m\in\mathcal{D}}(-1)^{\sigma_0}h_{l,m}}\frac{\prod_{l<m,l,m\in\mathcal{D}}(r_l+r_m)}{\prod_{l\in\mathcal{D}}(r_l+(-1)^{\sigma_0}\alpha_{\tilde{q}_l})}, \tag{56}$$

where

$$\tilde{c}_n = ((-1)^{\sigma_0} - ab)(\boldsymbol{\alpha\beta})^{(1-n)/2}.$$

Analogously, in the case of even n and $\sigma_0 = \sigma_\pi$, using (39) we get the same formula (56) for the matrix elements but with

$$\tilde{c}_n = (b + (-1)^{\sigma_0} a)\boldsymbol{\alpha}^{-1}(\boldsymbol{\alpha\beta})^{(2-n)/2}.$$

5. Product of matrix elements

In this section we sketch the calculation of the conjugate matrix elements $\langle\Phi_1|\sigma_n^z|\Phi_0\rangle$, where the vectors $\langle\Phi_1|$ and $|\Phi_0\rangle$ shall have the same eigenvalues as the vectors $|\Phi_1\rangle$ and $\langle\Phi_0|$ used in the previous sections. This calculation can be performed in the same way as we did in section 4. In analogy to (21), (22) we get for the homogeneous case

$$\frac{\langle\Phi_0|\sigma_n^z|\Phi_1\rangle}{\langle\tilde{\Psi}_{0,\mathbf{0}}|\tilde{\Psi}_{0,\mathbf{0}}\rangle} = \frac{a}{2r_0}\sum_{\boldsymbol{\rho}'}\mathcal{N}(\boldsymbol{\rho}')R_0^*(\boldsymbol{\rho}')R^*(\boldsymbol{\rho}')$$

with

$$R^*(\boldsymbol{\rho}') = \frac{t^{(1)}(-\zeta)}{\prod_{l=1}^{n-1}(-\zeta + (-1)^{\rho_l}r_l)} + \frac{t^{(0)}(\zeta)}{\prod_{l=1}^{n-1}(\zeta + (-1)^{\rho_l}r_l)}.$$

Now we have to make the same transformations as we made for $R(\boldsymbol{\rho}')$ in section 4.1. The expression for $R^*(\boldsymbol{\rho}')$ is obtained from $R(\boldsymbol{\rho}')$ given by (22) just by substituting $b \to -b$ (in particular, $\zeta \to -\zeta$). Let us compare $R_0^*(\boldsymbol{\rho}')$ and $R_0(\boldsymbol{\rho}')$. From the solution of the Baxter equations it follows that

$$Q_l^{\mathrm{L}(1)}(\rho_l)Q_l^{\mathrm{R}(0)}(\rho_l) = Q_l^{\mathrm{L}(0)}(\rho_l)Q_l^{\mathrm{R}(1)}(\rho_l) \qquad \text{unless} \qquad l \in \mathcal{D} \quad \text{and} \quad \rho_l = 1.$$

$$Q_l^{\mathrm{L}(1)}(1)Q_l^{\mathrm{R}(0)}(1) = -Q_l^{\mathrm{L}(0)}(1)Q_l^{\mathrm{R}(1)}(1) \qquad \text{if} \qquad l \in \mathcal{D}.$$

So, in the final formula we have to substitute $\tilde{q}_l \to -\tilde{q}_l$.

Using these rules, in the case of $\sigma_0 = \sigma_\pi$, from (56) we get

$$\frac{\langle\Phi_1|\sigma_n^z|\Phi_0\rangle}{\langle\tilde{\Psi}_{0,\mathbf{0}}|\tilde{\Psi}_{0,\mathbf{0}}\rangle} = r_0\tilde{c}_n c_\alpha \prod_{k\in\check{\mathcal{D}}}(-(-1)^k b + ar_k)$$
$$\times \frac{\prod_{l\in\mathcal{D}} 2r_l\, \mathrm{e}^{-\mathrm{i}\tilde{q}_l}(f_l^*)^{(D-1)/2}(g_l^*)^{(D-3)/2}}{\prod_{l<m,l,m\in\mathcal{D}}(-1)^{\sigma_0}h_{l,m}^*}\frac{\prod_{l<m,l,m\in\mathcal{D}}(r_l + r_m)}{\prod_{l\in\mathcal{D}}(r_l + (-1)^{\sigma_0}\alpha_{-\tilde{q}_l})}, \tag{57}$$

where $h_{l,m}^*$, f_l^*, g_l^* are $h_{l,m}$, f_l, g_l from (54) with the replacement $\tilde{q}_l \to -\tilde{q}_l$.

In the product of (56) with (57) nice simplifications appear. We use

$$\prod_{k\in\check{\mathcal{D}}}((-1)^k b + ar_k)(-(-1)^k b + ar_k) = \prod_{k\in\check{\mathcal{D}}}\frac{\boldsymbol{\alpha\beta}}{A(\tilde{q}_l)}, \tag{58}$$

and $f_l \cdot f_l^* = g_l \cdot g_l^* = A(\tilde{q}_l)$, so that

$$\frac{\langle\Phi_0|\sigma_n^z|\Phi_1\rangle}{\langle\tilde{\Psi}_{0,\mathbf{0}}|\tilde{\Psi}_{0,\mathbf{0}}\rangle}\frac{\langle\Phi_1|\sigma_n^z|\Phi_0\rangle}{\langle\tilde{\Psi}_{0,\mathbf{0}}|\tilde{\Psi}_{0,\mathbf{0}}\rangle} = \tilde{c}_n\tilde{c}_n^* r_0^2(c_\alpha)^2\prod_{k\in\check{\mathcal{D}}}\frac{\boldsymbol{\alpha\beta}}{A(\tilde{q}_k)}$$
$$\times\prod_{l\in\mathcal{D}}\left(\frac{4r_l^2 A(\tilde{q}_l)^{D-2}}{(r_l + (-1)^{\sigma_0}\alpha_{\tilde{q}_l})(r_l + (-1)^{\sigma_0}\alpha_{-\tilde{q}_l})}\prod_{\substack{m>l\\ m\in\mathcal{D}}}\frac{(r_l + r_m)^2}{|h_{l,m}|^2}\right), \tag{59}$$

where $\tilde{c}_n^*$ is $\tilde{c}_n$ with $b \to -b$ and $\tilde{c}_n\tilde{c}_n^* = \boldsymbol{\alpha}^{1-n}\boldsymbol{\beta}^{2-n}$ is independent of parity of n. Using further (45) and the short notations: $\lambda_0 = (-1)^{\sigma_0} s_0$, $\lambda_\pi = (-1)^{\sigma_\pi} s_\pi$ with $\sigma_0 = \sigma_\pi$

$$|h_{l,m}|^2 = 2(\cos\tilde{q}_m - \cos\tilde{q}_l)\frac{\sin\frac{1}{2}(\tilde{q}_l + \tilde{q}_m)}{\sin\frac{1}{2}(\tilde{q}_l - \tilde{q}_m)} = \frac{r_l^2 - r_m^2}{-\boldsymbol{\alpha\beta}} A(\tilde{q}_m)A(\tilde{q}_l)\frac{\sin\frac{1}{2}(\tilde{q}_l + \tilde{q}_m)}{\sin\frac{1}{2}(\tilde{q}_l - \tilde{q}_m)},$$

$$\frac{\lambda_\pi - \lambda_0}{\lambda_\pi + \lambda_0} = -\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}, \qquad 2r_l(r_l + \lambda_0)(r_l + \lambda_\pi) = (\lambda_0 + \lambda_\pi)\big(r_l + (-1)^{\sigma_0}\alpha_{\tilde{q}_l}\big)\big(r_l + (-1)^{\sigma_0}\alpha_{-\tilde{q}_l}\big),$$

we find that in (59) the factors $A(\tilde{q}_l)$ combine to

$$\prod_{k\in\check{\mathcal{D}}} \frac{1}{A(\tilde{q}_k)} \prod_{l\in\mathcal{D}} \left(A(\tilde{q}_l)^{D-2} \prod_{m>l,m\in\mathcal{D}} \frac{1}{A(\tilde{q}_m)A(\tilde{q}_l)} \right) = \prod_{l\in\check{\mathcal{D}}\cup\mathcal{D}} \frac{1}{A(\tilde{q}_l)} = \frac{\boldsymbol{\alpha}}{r_0^2}. \tag{60}$$

Since also the factors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ in (59) can be collected as follows ($|\check{\mathcal{D}}| + D = n - 1$):

$$\tilde{c}_n\tilde{c}_n^*(c_\alpha)^2(\boldsymbol{\alpha\beta})^{|\check{\mathcal{D}}|}(-\boldsymbol{\alpha\beta})^{D(D-1)/2}\boldsymbol{\alpha} = (-\boldsymbol{\alpha}/\boldsymbol{\beta})^{(D-1)/2},$$

we get finally for arbitrary n and $\sigma_0 = \sigma_\pi$

$$\frac{\langle\Phi_0|\sigma_n^z|\Phi_1\rangle\langle\Phi_1|\sigma_n^z|\Phi_0\rangle}{\langle\tilde{\Psi}_{0,\mathbf{0}}|\tilde{\Psi}_{0,\mathbf{0}}\rangle^2} = \big(\lambda_\pi^2 - \lambda_0^2\big)^{(D-\delta)/2}(\lambda_0 + \lambda_\pi)^\delta \prod_{l\in\mathcal{D}} \frac{2r_l}{(\lambda_0 + r_l)(\lambda_\pi + r_l)}$$
$$\times \prod_{l<m,l,m\in\mathcal{D}} \frac{r_l + r_m}{r_l - r_m} \cdot \frac{\sin\frac{1}{2}(\tilde{q}_l - \tilde{q}_m)}{\sin\frac{1}{2}(\tilde{q}_l + \tilde{q}_m)} \tag{61}$$

where $\delta = 1$. In a similar way we can find the product of matrix elements in the case of $\sigma_0 \neq \sigma_\pi$. The final result is (61) with $\delta = 0$. Observe that using (61), the explicit appearance of excitations of type (ii), i.e. $k \in \check{\mathcal{D}}$ has disappeared from our formula (recall that we still exclude $k \in \widehat{\mathcal{D}}$). We still have normalized our matrix elements by the norm taken from the auxiliary system. In the following section we shall normalize to the norm of periodic states so that the spin matrix element becomes independent of the special normalization of the periodic states chosen. We shall also include the hitherto excluded case (iii).

6. Final formula for the square of the matrix element

The proper quantity to consider for the matrix element of the spin operator, which does not depend on the normalization of the eigenvectors of the transfer matrix, is

$$\langle\Phi_0|\sigma_n^z|\Phi_1\rangle\langle\Phi_1|\sigma_n^z|\Phi_0\rangle/(\langle\Phi_0|\Phi_0\rangle\langle\Phi_1|\Phi_1\rangle). \tag{62}$$

The factor

$$\langle\Phi_0|\Phi_0\rangle\langle\Phi_1|\Phi_1\rangle/\langle\tilde{\Psi}_{0,\mathbf{0}}|\tilde{\Psi}_{0,\mathbf{0}}\rangle^2 \tag{63}$$

providing this change of normalization has been derived in formulae (74) and (75) of [2] for odd and even n, respectively. To obtain (62) we just divide (61) by (63). The final result for the square of the matrix element (61) as well as the formulae for the squares of norm (63) were obtained for the eigenvectors with eigenvalues not containing factors $(\lambda - s_{q_k})^2$, i.e. up to now we have excluded the case (iii) in section 3.2.

6.1. Excitations $j \in \widehat{\mathcal{D}}$ producing factors $(\lambda - s_{q_j})^2$ in $t^{(\rho)}(\lambda)$

Now we explain how to modify these formulae for the matrix elements and norms if the eigenvalue polynomials of states $|\Phi_0\rangle$ and $|\Phi_1\rangle$ contain factors $(\lambda - s_{q_j})^2$ for some j, so that $t^{(\rho)}(r_j) = 0$ for ρ satisfying $(-1)^{\rho} = (-1)^{j-1}$. We denote the set of such j, corresponding to both states $|\Phi_0\rangle$ and $|\Phi_1\rangle$, by $\widehat{\mathcal{D}}$. As already mentioned in section 3.2, case (iii), we cannot normalize the solution to the Baxter equation for the state $|\Phi_\rho\rangle$ by $Q_j^{\mathrm{L,R}(\rho)}(0) = 1$. However, we may normalize it by $Q_j^{\mathrm{L,R}(\rho)}(1) = 1$. For the other state, the solution to the Baxter equation is managed by the case (i) and there is no problem with the normalization $Q_j^{\mathrm{L,R}(\rho)}(0) = 1$. We shall use the normalization $Q_j^{\mathrm{L,R}(\rho)}(1) = 1$ for all $j \in \widehat{\mathcal{D}}$ irrespective of whether we have case (i) or (iii).

In [2] the norm (56) and the matrix element (21) were calculated using the normalization $Q_j^{\mathrm{L,R}(\rho)}(0) = 1$ for all $j = 1, 2, \ldots, n-1$. These formulae were obtained for the case of generic parameters for which any normalization is possible. Let us trace the changes in these formulae if instead we choose the normalization $Q_j^{\mathrm{L,R}(\rho)}(1) = 1$ for j from a subset $\widehat{\mathcal{D}} \subset \{1, 2, \ldots, n-1\}$.

Compare the formulae for the matrix element (21) corresponding to a different normalization of the solutions to the Baxter equation, i.e. we compare the term corresponding to a set $\boldsymbol{\rho}'$ in one formula with the term corresponding to the set $\boldsymbol{\rho}'^{+\widehat{\mathcal{D}}}$ in the other formula (the set $\boldsymbol{\rho}'^{+\widehat{\mathcal{D}}}$ is obtained from the set $\boldsymbol{\rho}'$ by shifts $\rho_j \to \rho_j + 1$, $j \in \widehat{\mathcal{D}}$). For $N = 2$ this just means interchanging $\rho_j = 0$ and $\rho_j = 1$, while the other components remain unchanged. Also, we change all $r_j \to -r_j$, $j \in \widehat{\mathcal{D}}$ in the second formula.

From the Baxter equations (7) and (8), the solution $Q_j^{\mathrm{L,R}(\rho)}(\rho_j + 1)$ normalized by $Q_j^{\mathrm{L,R}(\rho)}(1) = 1$ coincides with $Q_j^{\mathrm{L,R}(\rho)}(\rho_j)\big|_{r_j \to -r_j}$ with the normalization $Q_j^{\mathrm{L,R}(\rho)}(0) = 1$. The only factor which is changing in (21) is $\mathcal{N}(\boldsymbol{\rho}')$. The denominator is unchanged under the simultaneous substitutions $r_j \to -r_j$ and $\rho_j \to \rho_j + 1$. The change in the numerator is corrected by the division of the matrix elements corresponding to solutions of Baxter equations with $Q_k^{\mathrm{L,R}(\rho)}(1) = 1$, not by $\langle \tilde{\Psi}_{0,\mathbf{0}} | \tilde{\Psi}_{0,\mathbf{0}} \rangle$ but by $\langle \tilde{\Psi}_{0,\mathbf{0}^{+\widehat{\mathcal{D}}}} | \tilde{\Psi}_{0,\mathbf{0}^{+\widehat{\mathcal{D}}}} \rangle$. From the general expression for the norm, (20) of [2] at $N = 2$, the change of normalization means multiplying our matrix elements by

$$\frac{\langle \tilde{\Psi}_{0,\mathbf{0}} | \tilde{\Psi}_{0,\mathbf{0}} \rangle}{\langle \tilde{\Psi}_{0,\mathbf{0}^{+\widehat{\mathcal{D}}}} | \tilde{\Psi}_{0,\mathbf{0}^{+\widehat{\mathcal{D}}}} \rangle} = \frac{\prod_{l<m}^{n-1} (r_m + r_l)}{\prod_{l<m}^{n-1} (r_m (-1)^{\rho_m} + r_l (-1)^{\rho_l})}, \tag{64}$$

where $\rho_m = 1$ if $m \in \widehat{\mathcal{D}}$ and $\rho_m = 0$ otherwise. Finally, the factor $(-1)^{n\tilde{\rho}'}$ gives the sign $(-1)^{|\widehat{\mathcal{D}}|n}$. The formula for the norms undergoes the same changes. Therefore formally the expression (62) has to be invariant with respect to the substitutions $r_j \to -r_j$. But the final formula for (62) is given for the case of Ising model where we already replaced the dependence on s_{q_j} using the coincidence with r_j. So the substitutions $r_j \to -r_j$ in this final expression for (62) given in terms of λ_0, λ_π and r_k, $k = 1, 2, \ldots, n-1$, will also change the eigenvectors entering (62) to the eigenvectors corresponding to eigenvalue polynomials with factors $(\lambda - r_j)^2$, $j \in \widehat{\mathcal{D}}$, instead of $(\lambda + r_j)^2$. This is exactly what we need.

Summarizing: the final result (62) was obtained for eigenvectors with eigenvalues not containing factors $(\lambda - s_{q_j})^2$ and which could be given in terms of λ_0, λ_π and $r_k, k = 1, 2, \ldots, n-1$. Now, if the eigenvalue polynomial contains the factors $(\lambda - s_{q_j})^2$ instead of $(\lambda + s_{q_j})^2$ for some j, we just have to replace $r_j \to -r_j$ in the final formula for all such j.

6.2. *Final result in terms of* λ_0, λ_π, r_k *and* $\tilde{q}_l$

So the final formula for the matrix element becomes

$$\frac{\langle\Phi_0|\sigma_n^z|\Phi_1\rangle\langle\Phi_1|\sigma_n^z|\Phi_0\rangle}{\langle\Phi_0|\Phi_0\rangle\langle\Phi_1|\Phi_1\rangle} = \left(\lambda_\pi^2 - \lambda_0^2\right)^{(D-\delta)/2}(\lambda_0+\lambda_\pi)^\delta \prod_{\substack{l<m\\ l,m\in\mathcal{D}}} \left(\frac{r_l+r_m}{r_l-r_m}\cdot\frac{\sin\frac{1}{2}(\tilde{q}_l-\tilde{q}_m)}{\sin\frac{1}{2}(\tilde{q}_l+\tilde{q}_m)}\right)$$
$$\times\frac{\Lambda_n}{2^D\prod_{k\in\overline{\mathcal{D}}}(\dot{+}2r_k)}\cdot\frac{\prod_{k\,\mathrm{odd},l\,\mathrm{even}}((\dot{-}r_k\dot{+}r_l)(\dot{+}r_k\dot{-}r_l))}{\prod_{k<l,k,l\,\mathrm{odd}}((\dot{+}r_k\dot{+}r_l)(\dot{-}r_k\dot{-}r_l))\prod_{k<l,k,l\,\mathrm{even}}((\dot{+}r_k\dot{+}r_l)(\dot{-}r_k\dot{-}r_l))}, \qquad (65)$$

where

$$\Lambda_n = \frac{\prod_{k\in\overline{\mathcal{D}}^{(0)}}(\lambda_0\dot{+}r_k)}{\prod_{k\in\overline{\mathcal{D}}^{(1)}}(\lambda_0\dot{+}r_k)\prod_{k\in\mathcal{D}^{(1)}}\left(\lambda_0^2-r_k^2\right)}\cdot\frac{\prod_{k\in\overline{\mathcal{D}}^{(1)}}(\lambda_\pi\dot{+}r_k)}{\prod_{k\in\overline{\mathcal{D}}^{(0)}}(\lambda_\pi\dot{+}r_k)\prod_{k\in\mathcal{D}^{(0)}}\left(\lambda_\pi^2-r_k^2\right)}, \qquad \text{for odd } n,$$
$$\Lambda_n = \frac{\prod_{k\in\overline{\mathcal{D}}^{(0)}}(\lambda_0\dot{+}r_k)(\lambda_\pi\dot{+}r_k)}{(\lambda_0+\lambda_\pi)\prod_{k\in\overline{\mathcal{D}}^{(1)}}(\lambda_0\dot{+}r_k)(\lambda_\pi\dot{+}r_k)\prod_{k\in\mathcal{D}^{(1)}}\left(\lambda_0^2-r_k^2\right)\left(\lambda_\pi^2-r_k^2\right)}, \qquad \text{for even } n,$$

$\overline{\mathcal{D}} = \breve{\mathcal{D}}\cup\widehat{\mathcal{D}}$, $\overline{\mathcal{D}}^{(0)} = \breve{\mathcal{D}}^{(0)}\cup\widehat{\mathcal{D}}^{(0)}$, $\overline{\mathcal{D}}^{(1)} = \breve{\mathcal{D}}^{(1)}\cup\widehat{\mathcal{D}}^{(1)}$ and $\dot{\pm} r_m$ is the short notation for r_m if $m\in\breve{\mathcal{D}}$, for $\pm\, r_m$ if $m\in\mathcal{D}$ and for $-r_m$ if $m\in\widehat{\mathcal{D}}$, respectively.

Recall the definitions of the various variables which appear in (65): the state vectors $\Phi_0\rangle$ and $\Phi_1\rangle$ are labelled by their excitation content. This is defined in (27)–(30), where also the explicit form of the zeros r_k of $B_n(\lambda)$ is given. $\tilde{q}_l$ is just q_l of (30) up to a sign, see (49). The special role of the quasi-momenta zero and π gives rise to the appearance of λ_0 and λ_π, see (28) and (29).

The right-hand side of the first line of (65) is just the right-hand side of (61) except for the last product in the first line of (61). The second line of (65) mainly is the change of normalization (63), given by (74) and (75) of [2]. However, it is slightly modified by a cancellation against the last product of the first line in (61). Also, we have taken into account the contributions of $k\in\widehat{\mathcal{D}}$: these have the same form as those for $k\in\breve{\mathcal{D}}$, just with reflected $r_k\to -r_k$ as discussed above.

We claim that these formulae prove the formula for the matrix element which was given in [4] in an equivalent version. In order to show the equivalence, in the following we perform some transformations of (65) to get a formula which is more appropriate for comparison.

6.3. *Final result in terms of momenta*

Let $\{\mathsf{q}_1,\mathsf{q}_2,\ldots,\mathsf{q}_K\}$ and $\{\mathsf{p}_1,\mathsf{p}_2,\ldots,\mathsf{p}_L\}$ be the sets of the momenta of the excitations presenting the states $|\Phi_0\rangle$ from the NS-sector and $|\Phi_1\rangle$ from the R-sector, respectively. After some lengthy but straightforward transformations of (65) we obtain

$$\frac{\langle\Phi_0|\sigma_n^z|\Phi_1\rangle\langle\Phi_1|\sigma_n^z|\Phi_0\rangle}{\langle\Phi_0|\Phi_0\rangle\langle\Phi_1|\Phi_1\rangle} = J(s_\pi+s_0)\left(s_\pi^2-s_0^2\right)^{(K+L-1)/2}\prod_{k=1}^{K}\frac{P^{\mathrm{NS}}_{\mathsf{q}_k}\prod_{\mathsf{q}\neq|\mathsf{q}_k|}^{\frac{\mathrm{NS}}{2}} N_{\mathsf{q},\mathsf{q}_k}}{\prod_{\mathsf{p}}^{\frac{\mathrm{R}}{2}} N_{\mathsf{p},\mathsf{q}_k}}$$
$$\times\prod_{l=1}^{L}\frac{P^{\mathrm{R}}_{\mathsf{p}_l}\prod_{\mathsf{p}\neq|\mathsf{p}_l|}^{\frac{\mathrm{R}}{2}} N_{\mathsf{p},\mathsf{p}_l}}{\prod_{\mathsf{q}}^{\frac{\mathrm{NS}}{2}} N_{\mathsf{q},\mathsf{p}_l}}\cdot\frac{\prod_{k=1}^{K}\prod_{l=1}^{L} M_{\mathsf{q}_k,\mathsf{p}_l}}{\prod_{k<k'}^{K} M_{\mathsf{q}_k,\mathsf{q}_{k'}}\prod_{l<l'}^{L} M_{\mathsf{p}_l,\mathsf{p}_{l'}}}, \qquad (66)$$

where NS/2 (R/2) is the subset of quasi-momenta from NS (R) taking values in the segment $0 < \mathsf{q} < \pi$, NS/2 (R/2) containing q_k with odd k (even k):

$$M_{\alpha,\beta} = \frac{s_\alpha + s_\beta}{s_\alpha - s_\beta} \cdot \frac{\sin\frac{\alpha+\beta}{2}}{\sin\frac{\alpha-\beta}{2}}, \qquad M_{\alpha,-\alpha} = \frac{s_\alpha^2\left(s_0^2 - s_\pi^2\right)}{\left(s_\pi^2 - s_\alpha^2\right)\left(s_0^2 - s_\alpha^2\right)},$$

$$N_{\alpha,\beta} = \frac{s_\alpha + s_\beta}{s_\alpha - s_\beta}, \qquad \mathcal{J} = \frac{\prod_{\mathsf{q}}^{\frac{\mathrm{NS}}{2}}(s_0 + s_\mathsf{q})}{\prod_{\mathsf{p}}^{\frac{\mathrm{R}}{2}}(s_0 + s_\mathsf{p})} \cdot \frac{\prod_{\mathsf{q}}^{\frac{\mathrm{NS}}{2}}\prod_{\mathsf{p}}^{\frac{\mathrm{R}}{2}}(s_\mathsf{q} + s_\mathsf{p})^2}{\prod_{\mathsf{q},\mathsf{q}'}^{\frac{\mathrm{NS}}{2}}(s_\mathsf{q} + s_{\mathsf{q}'})\prod_{\mathsf{p},\mathsf{p}'}^{\frac{\mathrm{R}}{2}}(s_\mathsf{p} + s_{\mathsf{p}'})}.$$

For n odd:

$$P_\mathsf{q}^{\mathrm{NS}} = \frac{s_\mathsf{q}}{(s_\pi - s_\mathsf{q})(s_0 + s_\mathsf{q})}, \qquad \mathsf{q} \neq \pi, \qquad P_\mathsf{p}^{\mathrm{R}} = \frac{s_\mathsf{p}}{(s_\pi + s_\mathsf{p})(s_0 - s_\mathsf{p})}, \qquad \mathsf{p} \neq 0,$$

$$P_0^{\mathrm{R}} = P_\pi^{\mathrm{NS}} = \frac{1}{s_\pi + s_0}, \qquad J = \frac{\prod_{\mathsf{p}}^{\frac{\mathrm{R}}{2}}(s_\pi + s_\mathsf{p})}{\prod_{\mathsf{q}}^{\frac{\mathrm{NS}}{2}}(s_\pi + s_\mathsf{q})}\mathcal{J},$$

for n even:

$$P_\mathsf{q}^{\mathrm{NS}} = \frac{s_\mathsf{q}}{(s_\pi + s_\mathsf{q})(s_0 + s_\mathsf{q})}, \qquad P_\mathsf{p}^{\mathrm{R}} = \frac{s_\mathsf{p}}{(s_\pi - s_\mathsf{p})(s_0 - s_\mathsf{p})}, \qquad \mathsf{p} \neq 0, \pi,$$

$$P_0^{\mathrm{R}} = -P_\pi^{\mathrm{NS}} = \frac{1}{s_\pi - s_0}, \qquad J = \frac{\prod_{\mathsf{p}}^{\frac{\mathrm{NS}}{2}}(s_\pi + s_\mathsf{q})}{\prod_{\mathsf{q}}^{\frac{\mathrm{R}}{2}}(s_\pi + s_\mathsf{p})}\mathcal{J}.$$

7. Bugrij–Lisovyy formula for matrix element

In [3, 4], the matrix elements of σ_k^z between eigenvectors of *symmetric* Ising transfer matrix

$$\mathbf{t}_{\mathrm{IsingSym}} = \exp\left(\frac{1}{2}\sum_{k=1}^{n} K_x\sigma_{k-1}^z\sigma_k^z\right)\exp\left(\sum_{k=1}^{n} K_x^*\sigma_k^x\right)\exp\left(\frac{1}{2}\sum_{k=1}^{n} K_x\sigma_{k-1}^z\sigma_k^z\right). \tag{67}$$

were given. Since (25) and (67) are related by a similarity transformation with

$$\exp\left(\frac{1}{2}\sum_{k=1}^{n} K_x\sigma_{k-1}^z\sigma_k^z\right),$$

which commutes with σ_m^z, it is natural to compare (66) with the square of the matrix element as given in [4]:

$$\begin{aligned}
&|_{\mathrm{NS}}\langle \mathsf{q}_1, \mathsf{q}_2, \ldots, \mathsf{q}_K|\sigma_m^z|\mathsf{p}_1, \mathsf{p}_2, \ldots, \mathsf{p}_L\rangle_{\mathrm{R}}|^2 \\
&\quad = \xi\xi_T \prod_{k=1}^{K} \frac{\prod_{\mathsf{q}\neq\mathsf{q}_k}^{\mathrm{NS}} \sinh\frac{\gamma(\mathsf{q}_k)+\gamma(q)}{2}}{n\prod_{\mathsf{p}}^{\mathrm{R}} \sinh\frac{\gamma(\mathsf{q}_k)+\gamma(\mathsf{p})}{2}} \prod_{l=1}^{L} \frac{\prod_{\mathsf{p}\neq\mathsf{p}_l}^{\mathrm{R}} \sinh\frac{\gamma(\mathsf{p}_l)+\gamma(\mathsf{p})}{2}}{n\prod_{\mathsf{q}}^{\mathrm{NS}} \sinh\frac{\gamma(\mathsf{p}_l)+\gamma(\mathsf{q})}{2}} \cdot \left(\frac{t_y - t_y^{-1}}{t_x - t_x^{-1}}\right)^{(K-L)^2/2} \\
&\quad\quad \times \prod_{k<k'}^{K} \frac{\sin^2\frac{\mathsf{q}_k-\mathsf{q}_{k'}}{2}}{\sinh^2\frac{\gamma(\mathsf{q}_k)+\gamma(\mathsf{q}_{k'})}{2}} \prod_{l<l'}^{L} \frac{\sin^2\frac{\mathsf{p}_l-\mathsf{p}_{l'}}{2}}{\sinh^2\frac{\gamma(\mathsf{p}_l)+\gamma(\mathsf{p}_{l'})}{2}} \prod_{\substack{1\leqslant k\leqslant K \\ 1\leqslant l\leqslant L}} \frac{\sinh^2\frac{\gamma(\mathsf{q}_k)+\gamma(\mathsf{p}_l)}{2}}{\sin^2\frac{\mathsf{q}_k-\mathsf{p}_l}{2}}.
\end{aligned} \tag{68}$$

In this formula the states are labelled by the momenta of the excitations, and the squared matrix element is given for σ_m^z, $m = 1, \ldots, n$. The operators σ_m^z with different values of m are related by similarity transformations with the translation operator. The states under consideration are eigenvectors of the translation operator [15] with eigenvalues which have unit absolute value. This explains why the formula presented does not depend on m. Therefore it is sufficient to calculate the matrix element for σ_n^z. The factors in front of the right-hand side of (68) are defined by

$$\xi = ((\sinh 2K_x \sinh 2K_y)^{-2} - 1)^{1/4}, \qquad \xi_T = \left(\frac{\prod_{\mathsf{q}}^{\mathrm{NS}} \prod_{\mathsf{p}}^{\mathrm{R}} \sinh^2 \frac{\gamma(\mathsf{q})+\gamma(\mathsf{p})}{2}}{\prod_{\mathsf{q},\mathsf{q}'}^{\mathrm{NS}} \sinh \frac{\gamma(\mathsf{q})+\gamma(\mathsf{q}')}{2} \prod_{\mathsf{p},\mathsf{p}'}^{\mathrm{R}} \sinh \frac{\gamma(\mathsf{p})+\gamma(\mathsf{p}')}{2}} \right)^{1/4},$$

where $\gamma(\mathsf{q})$ is the energy of the excitation with quasi-momentum q

$$\cosh \gamma(\mathsf{q}) = \frac{\left(t_x + t_x^{-1}\right)\left(t_y + t_y^{-1}\right)}{2\left(t_x^{-1} - t_x\right)} - \frac{t_y - t_y^{-1}}{t_x - t_x^{-1}} \cos \mathsf{q}, \tag{69}$$

where by (26) $t_x = \tanh K_x = ab$, $t_y = \tanh K_y = (a-b)/(a+b)$.

The excitation with quasi-momentum q leads to the multiplication of the transfer matrix eigenvalue by $\mathrm{e}^{-\gamma(\mathsf{q})}$ in the notations of [4], and in our notation to the multiplication by $\pm(\lambda - s_{\mathsf{q}})/(\lambda + s_{\mathsf{q}})$ at $\lambda = b/a$. The sign is not fixed because the excitations arise by pairs. Comparing (69) and (27) we get

$$\mathrm{e}^{\gamma(\mathsf{q})} = \frac{a s_{\mathsf{q}} + b}{a s_{\mathsf{q}} - b}. \tag{70}$$

Therefore

$$\sinh \tfrac{1}{2}(\gamma(\alpha) + \gamma(\beta)) = \mathrm{e}^{\frac{1}{2}(\gamma(\alpha)+\gamma(\beta))} \frac{ab(s_\alpha + s_\beta)}{(b + a s_\alpha)(b + a s_\beta)}, \tag{71}$$

which leads, in particular, to

$$\frac{\sinh \frac{\gamma(\alpha_1)+\gamma(\alpha_2)}{2} \cdot \sinh \frac{\gamma(\alpha_3)+\gamma(\alpha_4)}{2}}{\sinh \frac{\gamma(\alpha_1)+\gamma(\alpha_3)}{2} \cdot \sinh \frac{\gamma(\alpha_2)+\gamma(\alpha_4)}{2}} = \frac{\left(s_{\alpha_1} + s_{\alpha_2}\right)\left(s_{\alpha_3} + s_{\alpha_4}\right)}{\left(s_{\alpha_1} + s_{\alpha_3}\right)\left(s_{\alpha_2} + s_{\alpha_4}\right)}. \tag{72}$$

Our next problem is to rewrite (68) in terms of s_{q}. We need

$$\xi \left(\frac{\sinh^2 \frac{\gamma(0)+\gamma(\pi)}{2}}{\sinh \gamma(0) \sinh \gamma(\pi)} \right)^{1/4} = \frac{1}{(\sinh 2K_x \sinh 2K_y)^{1/2}},$$

$$\frac{t_y - t_y^{-1}}{t_x - t_x^{-1}} = \frac{\sinh 2K_x}{\sinh 2K_y}, \qquad \sinh \frac{\gamma(0) + \gamma(\pi)}{2} = \frac{1}{\sinh 2K_y}.$$

The following formulae give a correspondence between different parts of (68) and (66):

$$\frac{\xi \xi_T}{\sinh \frac{1}{2}(\gamma(0) + \gamma(\pi))} \left(\frac{t_y - t_y^{-1}}{t_x - t_x^{-1}} \right)^{1/2} = J,$$

$$\frac{\prod_{\mathsf{q}\neq\mathsf{q}_k}^{\mathrm{NS}} \sinh \frac{\gamma(\mathsf{q}_k)+\gamma(\mathsf{q})}{2}}{n \prod_{\mathsf{p}}^{\mathrm{R}} \sinh \frac{\gamma(\mathsf{q}_k)+\gamma(\mathsf{p})}{2}} = \frac{s_0 + s_\pi}{\sinh \frac{\gamma(0)+\gamma(\pi)}{2}} \frac{P_{\mathsf{q}_k}^{\mathrm{NS}} \prod_{\mathsf{q}\neq|\mathsf{q}_k|}^{\frac{\mathrm{NS}}{2}} N_{\mathsf{q},\mathsf{q}_k}}{\prod_{\mathsf{p}}^{\frac{\mathrm{R}}{2}} N_{\mathsf{p},\mathsf{q}_k}},$$

$$\frac{\prod_{\mathsf{p}\neq\mathsf{p}_l}^{\mathrm{R}} \sinh \frac{\gamma(\mathsf{p}_l)+\gamma(\mathsf{p})}{2}}{n \prod_{\mathsf{q}}^{\mathrm{NS}} \sinh \frac{\gamma(\mathsf{p}_j)+\gamma(\mathsf{q})}{2}} = \frac{s_0 + s_\pi}{\sinh \frac{\gamma(0)+\gamma(\pi)}{2}} \frac{P_{\mathsf{p}_l}^{\mathrm{R}} \prod_{\mathsf{p}\neq|\mathsf{p}_l|}^{\frac{\mathrm{R}}{2}} N_{\mathsf{p},\mathsf{p}_l}}{\prod_{\mathsf{q}}^{\frac{\mathrm{NS}}{2}} N_{\mathsf{q},\mathsf{p}_l}},$$

where in the last two formulae we used

$$\sinh^2 \tfrac{1}{2}(\gamma(\alpha) + \gamma(\beta)) = -\frac{t_y - t_y^{-1}}{t_x - t_x^{-1}} \cdot \frac{s_\alpha + s_\beta}{s_\alpha - s_\beta} \cdot \sin \tfrac{1}{2}(\alpha - \beta) \cdot \sin \tfrac{1}{2}(\alpha + \beta), \tag{73}$$

and, in particular,

$$\sinh^2 \tfrac{1}{2}(\gamma(0) + \gamma(\pi)) = \frac{t_y - t_y^{-1}}{t_x - t_x^{-1}} \cdot \frac{s_0 + s_\pi}{s_0 - s_\pi}, \tag{74}$$

together with (72) and some trigonometric identities. Formula (73) also gives

$$\frac{\sinh^2\frac{\gamma(\alpha)+\gamma(\beta)}{2}}{\sin^2\frac{\alpha-\beta}{2}} = -\frac{t_y - t_y^{-1}}{t_x - t_x^{-1}} M_{\alpha,\beta}. \tag{75}$$

Formula (75) is also valid for $\beta = -\alpha$, but in this case we have to use formulae (70) and (71). Finally, if we take into account (74) and that K in (66) is even, L is odd, then it is easy to see that formulae (66) and (68) coincide.

8. Matrix elements for the quantum Ising chain in a transverse field

In this section we apply the formulae for the matrix elements obtained in section 6 to the derivation of the matrix elements for the quantum Ising chain in a transverse field. Let us start from the L-operator (24) with $a = g^{-1/2}$ and $b = 0$:

$$L_k(\lambda) = \begin{pmatrix} 1 + \lambda\sigma_k^x & \lambda g^{-1/2}\sigma_k^z \\ g^{-1/2}\sigma_k^z & \lambda g^{-1} \end{pmatrix}. \tag{76}$$

Expanding the transfer matrix for the monodromy matrix (2) with this L-operator we have:

$$\mathbf{t}_n(\lambda) = \mathbf{1} - \frac{2\lambda}{g}\hat{\mathcal{H}} + \cdots, \qquad \hat{\mathcal{H}} = -\frac{1}{2}\sum_{k=1}^{n}\left(\sigma_k^z\sigma_{k+1}^z + g\sigma_k^x\right),$$

where $\hat{\mathcal{H}}$ is the Hamiltonian of the periodic quantum Ising chain in a transverse field. From (27) we get the spectrum of this Hamiltonian

$$\mathcal{E} = -\frac{1}{2}\sum_{\mathsf{q}} \pm\varepsilon(\mathsf{q}), \tag{77}$$

where the energies of the quasi-particle excitations are

$$\varepsilon(\mathsf{q}) = (1 - 2g\cos\mathsf{q} + g^2)^{1/2} = \left((g-1)^2 + 4g\sin^2\frac{\mathsf{q}}{2}\right)^{1/2}, \qquad \mathsf{q} \neq 0, \pi,$$

$$\varepsilon(0) = g - 1, \qquad \varepsilon(\pi) = g + 1.$$

In (77), the sign $+/-$ in front of $\varepsilon(\mathsf{q})$ corresponds to the absence/presence of the excitation with the momentum q. The NS-sector includes the states with an even number of excitations, the R-sector includes the states with an odd number of excitations. The momentum q runs over the same set as in (27). Then the formula for matrix elements for σ_n^z is given by (66) with $s_{\mathsf{q}} = g/\varepsilon(\mathsf{q})$. After some simplification we get the analogue of (68) now for the quantum Ising chain:

$$|_{\mathrm{NS}}\langle \mathsf{q}_1, \mathsf{q}_2, \ldots, \mathsf{q}_K|\sigma_m^z|\mathsf{p}_1, \mathsf{p}_2, \ldots, \mathsf{p}_L\rangle_{\mathrm{R}}|^2 = g^{\frac{(K-L)^2}{2}}\xi\xi_T\prod_{k=1}^{K}\frac{\mathrm{e}^{\eta(\mathsf{q}_k)}}{n\varepsilon(\mathsf{q}_k)}\prod_{l=1}^{L}\frac{\mathrm{e}^{-\eta(\mathsf{p}_l)}}{n\varepsilon(\mathsf{p}_l)}$$
$$\times\prod_{k<k'}^{K}\left(\frac{2\sin\frac{\mathsf{q}_k-\mathsf{q}_{k'}}{2}}{\varepsilon(\mathsf{q}_k)+\varepsilon(\mathsf{q}_{k'})}\right)^2\prod_{l<l'}^{L}\left(\frac{2\sin\frac{\mathsf{p}_l-\mathsf{p}_{l'}}{2}}{\varepsilon(\mathsf{p}_l)+\varepsilon(\mathsf{p}_{l'})}\right)^2\prod_{k=1}^{K}\prod_{l=1}^{L}\left(\frac{\varepsilon(\mathsf{p}_l)+\varepsilon(\mathsf{q}_k)}{2\sin\frac{\mathsf{p}_l-\mathsf{q}_k}{2}}\right)^2, \tag{78}$$

where

$$\xi = (g^2-1)^{\frac{1}{4}}, \qquad \xi_T = \frac{\prod_{\mathsf{q}}^{\mathrm{NS}}\prod_{\mathsf{p}}^{\mathrm{R}}(\varepsilon(\mathsf{q})+\varepsilon(\mathsf{p}))^{\frac{1}{2}}}{\prod_{\mathsf{q},\mathsf{q}'}^{\mathrm{NS}}(\varepsilon(\mathsf{q})+\varepsilon(\mathsf{q}'))^{\frac{1}{4}}\prod_{\mathsf{p},\mathsf{p}'}^{\mathrm{R}}(\varepsilon(\mathsf{p})+\varepsilon(\mathsf{p}'))^{\frac{1}{4}}}$$

and

$$e^{\eta(\mathsf{q})} = \frac{\prod_{\mathsf{q}'}^{\mathrm{NS}} \left(\varepsilon(\mathsf{q}) + \varepsilon(\mathsf{q}')\right)}{\prod_{\mathsf{p}}^{\mathrm{R}} \left(\varepsilon(\mathsf{q}) + \varepsilon(\mathsf{p})\right)}.$$

Formally, all these formulae are correct for the paramagnetic phase where $g > 1$ and for the ferromagnetic phase where $0 \leqslant g < 1$. But for the case $0 \leqslant g < 1$ it is natural to redefine the energy of zero-momentum excitation as $\varepsilon(0) = 1 - g$ to be positive. From (77), this change of the sign of $\varepsilon(0)$ in the ferromagnetic phase leads to a formal change between absence–presence of zero-momentum excitation in the labelling of eigenstates. Therefore the number of the excitations in each sector (NS and R) becomes even. Direct calculation shows that the change of the sign of $\varepsilon(0)$ in (78) can be absorbed to obtain formally the same formula (78) but with new $\varepsilon(0)$, even L (the number of the excitations in R-sector) and new $\xi = (1-g^2)^{1/4}$.

Formulae (68) and (78) allow us to reobtain already known formulae for the Ising model, e.g. the spontaneous magnetization [16, 17]. Indeed, for the quantum Ising chain in the ferromagnetic phase ($0 \leqslant g < 1$) and in the thermodynamic limit $n \to \infty$ (when the energies of $|\mathrm{vac}\rangle_{\mathrm{NS}}$ and $|\mathrm{vac}\rangle_{\mathrm{R}}$ coincide giving the degeneration of the ground state), we have $\xi_T \to 1$ and therefore the spontaneous magnetization ${}_{\mathrm{NS}}\langle \mathrm{vac}|\sigma_m^z|\mathrm{vac}\rangle_{\mathrm{R}} = \xi^{1/2} = (1-g^2)^{1/8}$.

9. Conclusions

In this paper we calculated the normalized spin matrix element between arbitrary states of the Ising model, the main result being the formulae (65), (66) and (78). We started with the result (12) obtained in our previous paper [2] using the Sklyanin method of separation of variables by which we obtained explicit wavefunctions in terms of the solutions of Baxter equations. The result (12) was obtained for the general $N = 2$ BBS model which is related to a generalized free-fermion Ising-type model (3). For this general model we were able to get the much simpler formula (21) which however still involves a multiple sum over intermediate spins. Since for the general model we cannot perform the summation, for the further calculation we restricted ourselves to the Ising model with parameters (23). Performing a number of technical manipulations, we succeed in calculating the multiple spin sums explicitly. Although the intermediate formulae are quite involved, a number of surprising cancellations take place which lead to the rather simple formula (61) for the spin matrix element square. This comes still normalized to the auxiliary states involved in the method of separation of variables, but it is not difficult to convert this result into the properly normalized matrix elements for the model with periodic boundary condition. The final formula becomes more lengthy due to normalization factors. We show by which transformations we get the recently conjectured formula of Bugrij and Lisovyy. Our derivation provides a first proof of these formulae. Another application of the formulae obtained in this paper is the result (78) for the spin matrix elements for the finite quantum Ising chain in a transverse field.

The presence of degenerations in the spectrum for the special Ising parameter values forced us in this case to normalize the Baxter equation solutions differently for different excited states. The complexity of the formulae gives little hope that for more general parameter values the multiple spin summations can be done in the near future, even if then the degeneration problems may be avoided.

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Appendix. Proof of the summation formula

The aim of this appendix is to find a factorized expression for the sum

$$Y_{\mathcal{D}} = \sum_{\rho_l, l\in\mathcal{D}} \frac{\prod_{l\in\mathcal{D}}(-1)^{\rho_l}((-1)^{\rho_l}r_l + \xi_l)((-1)^{\rho_l}r_l + \zeta)}{\prod_{l<m,l,m\in\mathcal{D}}((-1)^{\rho_l}r_l + (-1)^{\rho_m}r_m)} \tag{A.1}$$

where ξ_l is given by (49) with (47). The result for $\xi_l = \pm\alpha_{\tilde{q}_l}$ is

$$Y_{\mathcal{D}} = \sum_{\rho_l, l\in\mathcal{D}} \frac{\prod_{l\in\mathcal{D}}(-1)^{\rho_l}((-1)^{\rho_l}r_l \pm \alpha_{\tilde{q}_l})((-1)^{\rho_l}r_l + \zeta)}{\prod_{l<m,l,m\in\mathcal{D}}((-1)^{\rho_l}r_l + (-1)^{\rho_m}r_m)}$$

$$= \begin{cases} c_D^{\mathrm{odd}}(b\pm a)\left(\prod_{j\in\mathcal{D}} \mathrm{e}^{\mathrm{i}\tilde{q}_j} \mp ab\right) \dfrac{\prod_{l\in\mathcal{D}}(2r_l/a) f_l^{(D-1)/2} g_l^{(D-3)/2}}{\prod_{l,m\in\mathcal{D},l<m}(\pm h_{l,m})} & D \text{ odd} \\ c_D^{\mathrm{even}}(a\pm b)\left(a\prod_{j\in\mathcal{D}} \mathrm{e}^{\mathrm{i}\tilde{q}_j} \mp b\right) \dfrac{\prod_{l\in\mathcal{D}}(2r_l/a) (f_l g_l)^{D/2-1}}{\prod_{l,m\in\mathcal{D},l<m}(\pm h_{l,m})} & D \text{ even} \end{cases} \tag{A.2}$$

with $D = |\mathcal{D}|$,

$$c_D^{\mathrm{odd}} = \boldsymbol{\alpha}^{-(D-1)(D-3)/4}(-\boldsymbol{\beta})^{-(D-1)^2/4}, \qquad c_D^{\mathrm{even}} = \boldsymbol{\alpha}^{-(D-2)^2/4}(-\boldsymbol{\beta})^{-(D-2)D/4}, \tag{A.3}$$

and we use the abbreviations (54). Replacing $\pm\alpha_{\tilde{q}_l} \to \pm\beta_{\tilde{q}_l}$ in (A.2), see (47), (49), amounts to $\boldsymbol{\alpha} \leftrightarrow \boldsymbol{\beta}$ in c_D^{odd} and c_D^{even}, and

$$(b\pm a)\left(\prod_{j\in\mathcal{D}} \mathrm{e}^{\mathrm{i}\tilde{q}_j} \mp ab\right) \to (1\mp ab)\left(b\prod_{j\in\mathcal{D}} \mathrm{e}^{\mathrm{i}\tilde{q}_j} \pm a\right) \qquad D \text{ odd},$$

$$(a\pm b)\left(a\prod_{j\in\mathcal{D}} \mathrm{e}^{\mathrm{i}\tilde{q}_j} \mp b\right) \to (1\mp ab)\left(\pm ab\prod_{j\in\mathcal{D}} \mathrm{e}^{\mathrm{i}\tilde{q}_j} + 1\right) \qquad D \text{ even}.$$

In section 4.3 the last bracket in the numerator of (A.1) is also needed with $+\zeta = b/a$ replaced by $-\zeta$. However, in order not to complicate the formulae, we shall always use (A.1) as it is written here. Since the only other b-dependence, which is in ξ_j and r_j, is quadratic, this can be adjusted at the end of the calculation just by changing the sign of b. Also, it is sufficient to prove formula (A.2) for the case $\xi_l = \alpha_{\tilde{q}_l}$. Then the results for the cases $\xi_l = -\alpha_{\tilde{q}_l}$ and $\xi_l = \pm\beta_{\tilde{q}_l}$ can be obtained by simple transformations of the variables r_l and b.

First, we find the recurrence relation for $Y_{\mathcal{D}}$ with respect to $D = |\mathcal{D}|$. It relates this quantity for D and $D-2$. Then we verify (A.2) for small D. Finally, by explicitly inserting our conjectured solutions (A.2) into the recursion relation we prove the expression. The cases of D odd and even have to be treated separately, since we are dealing with a two-step relation.

A.1. Derivation of the recursion relation

This recurrence relation for $Y_{\mathcal{D}}$ is obtained by using the identity, compare (17),

$$\sum_i \frac{\prod_k (x_i - y_k)}{\prod_{j\neq i}(x_i - x_j)} = 0, \tag{A.4}$$

when the number of x_i exceeds the number of y_k at least by two. Fix any index $s \in \mathcal{D}$ and consider $D+1$ values of x_i and two values of y_i: $\{y_1, y_2\} = \{-\xi_s, -\zeta\}$,

$$\{x_0, x_1, \ldots, x_D\} = \{r_s, -r_s, -(-1)^{\rho_1} r_1, -(-1)^{\rho_2} r_2, \ldots, \underbrace{-(-1)^{\rho_s} r_s}_{\text{omitted}}, \ldots, -(-1)^{\rho_D} r_D\}.$$

Since two parameters y_k are chosen, we must have $D \geqslant 3$. Now we separate the two terms in (A.4) which correspond to $i = 0, 1$ and present them as a summation over $\rho_s \in \{0, 1\}$ for $\{x_0, x_1\} = r_s(-1)^{\rho_s}$. Then (A.4) becomes

$$\sum_{\rho_s} \frac{(-1)^{\rho_s}(r_s(-1)^{\rho_s} + \xi_s)(r_s(-1)^{\rho_s} + \zeta)}{\prod_{k\neq s}(r_s(-1)^{\rho_s} + r_k(-1)^{\rho_k})}$$
$$= -\sum_{k\neq s} \frac{2r_s(-r_k(-1)^{\rho_k} + \xi_s)(-r_k(-1)^{\rho_k} + \zeta)}{\left(r_k^2 - r_s^2\right)\prod_{l\neq k,s}(-r_k(-1)^{\rho_k} + r_l(-1)^{\rho_l})}. \tag{A.5}$$

Now in (A.1) we separate the summation over a certain fixed discrete variable ρ_s and use the identity (A.5) to replace the summation over $\rho_s \in \{0, 1\}$ by a summation over k. After this, we move the summation over k to the front of formula (A.1) and collect the factors depending on ρ_k:

$$Y_{\mathcal{D}} = -\sum_{k\neq s} \sum_{\rho_{l\in\mathcal{D}/s,k}} \frac{\prod_{l\neq s,k}(-1)^{\rho_l}(r_l(-1)^{\rho_l} + \xi_l)(r_l(-1)^{\rho_l} + \zeta)}{\prod_{l<m,l,m\neq s,k}(r_l(-1)^{\rho_l} + r_m(-1)^{\rho_m})}$$
$$\times \sum_{\rho_k} \frac{(-1)^{\rho_k}(r_k(-1)^{\rho_k} + \xi_k)(r_k(-1)^{\rho_k} + \zeta)}{\prod_{l\neq k,s}(r_k(-1)^{\rho_k} + r_l(-1)^{\rho_l})} \frac{2r_s(-r_k(-1)^{\rho_k} + \xi_s)(-r_k(-1)^{\rho_k} + \zeta)}{\left(r_k^2 - r_s^2\right)\prod_{l\neq k,s}(-r_k(-1)^{\rho_k} + r_l(-1)^{\rho_l})}. \tag{A.6}$$

Now after multiplication in the second line of (A.6), we perform the summation over $\rho_k \in \{0, 1\}$ by means of the relation

$$\sum_{\rho_k} (-1)^{\rho_k}(r_k(-1)^{\rho_k} + \xi_k)(-r_k(-1)^{\rho_k} + \xi_s) = -2r_k(\xi_k - \xi_s).$$

Finally, we get the desired recursion relation, valid for any fixed index $s \in \mathcal{D}$:

$$Y_{\mathcal{D}} = \sum_{k\neq s} Y_{\mathcal{D}/k,s} \frac{4r_k r_s}{\left(r_k^2 - r_s^2\right)} \frac{\left(\zeta^2 - r_k^2\right)(\xi_k - \xi_s)}{\prod_{l\neq k,s}\left(r_l^2 - r_k^2\right)}, \tag{A.7}$$

where $Y_{\mathcal{D}/k,s}$ is just the original $Y_{\mathcal{D}}$ with the indices k and s removed from $\mathcal{D}$.

Since (A.7) is a two-step difference equation, in general it has two independent solutions $Y_{\mathcal{D}}^{(1)}$ and $Y_{\mathcal{D}}^{(2)}$. The quantity (A.1) is equal to a linear combination of these solutions, $Y_{\mathcal{D}} = c_1 Y_{\mathcal{D}}^{(1)} + c_2 Y_{\mathcal{D}}^{(2)}$ and the constants c_1, c_2 are fixed by calculating $Y_{\mathcal{D}}$ explicitly for small D.

In the following, using (A.7), we give the details of the proof of (A.2) for the case D odd. The derivation for D even proceeds analogously.

A.2. Proving the summation formula for D odd

For $D = 1$ we start calculating directly (A.1), $\alpha_s = \alpha_{\tilde{q}_s}$:

$$Y_{\{s\}} = \sum_{\rho_s} (-1)^{\rho_s}(r_s(-1)^{\rho_s} + \alpha_s)(r_s(-1)^{\rho_s} + b/a) = 2r_s \frac{(b+a)(\mathrm{e}^{\mathrm{i}\tilde{q}_s} - ab)}{a(\mathrm{e}^{\mathrm{i}\tilde{q}_s} - a^2)},$$

which proves (A.2) for this particular case. This result, together with the recursion relation (A.7), defines $Y_{\mathcal{D}}$ for odd D uniquely. For example, for the set $\mathcal{D} = \{s_1, s_2, s_3\}$, the recursion relation (A.7) with selected $s = s_3$ gives

$$\begin{aligned} Y_{\{s_1,s_2,s_3\}} &= Y_{\{s_2\}}\frac{4r_1r_3}{\left(r_1^2-r_3^2\right)}\frac{\left(\zeta^2-r_1^2\right)(\alpha_1-\alpha_3)}{\left(r_2^2-r_1^2\right)} + Y_{\{s_1\}}\frac{4r_2r_3}{\left(r_2^2-r_3^2\right)}\frac{\left(\zeta^2-r_2^2\right)(\alpha_2-\alpha_3)}{\left(r_1^2-r_2^2\right)} \\ &= \frac{(b+a)\prod_{l=1}^{3}(2r_l f_l)}{a^3(-\beta)\prod_{1\leqslant l<m\leqslant 3}h_{l,m}}\left(\frac{\mathrm{e}^{\mathrm{i}\tilde{q}_1}(\mathrm{e}^{\mathrm{i}\tilde{q}_2}-ab)h_{2,3}}{(\mathrm{e}^{\mathrm{i}\tilde{q}_2}-\mathrm{e}^{\mathrm{i}\tilde{q}_1})} + \frac{\mathrm{e}^{\mathrm{i}\tilde{q}_2}(\mathrm{e}^{\mathrm{i}\tilde{q}_1}-ab)h_{1,3}}{(\mathrm{e}^{\mathrm{i}\tilde{q}_1}-\mathrm{e}^{\mathrm{i}\tilde{q}_2})}\right) \\ &= \frac{(b+a)\prod_{l=1}^{3}(2r_l f_l)}{a^3(-\beta)\prod_{l<m}h_{l,m}}\left(\prod_{l=1}^{3}\mathrm{e}^{\mathrm{i}\tilde{q}_l}-ab\right), \end{aligned} \tag{A.8}$$

where we used

$$\alpha_k-\alpha_s = -\boldsymbol{\alpha}\rho_{k,s}, \qquad \zeta^2-r_k^2 = \frac{\boldsymbol{\alpha\beta}\,\mathrm{e}^{\mathrm{i}\tilde{q}_k}}{a^2 f_k g_k}, \qquad r_l^2-r_k^2 = \frac{\boldsymbol{\alpha\beta}h_{l,k}}{f_l f_k}\rho_{l,k} \tag{A.9}$$

with $\rho_{k,s} = (\mathrm{e}^{\mathrm{i}\tilde{q}_k}-\mathrm{e}^{\mathrm{i}\tilde{q}_s})/(g_k g_s)$. Observe that the big bracket in the second line of (A.8) factorizes and leads to a result symmetrical in the three indices. The result obtained in (A.8) proves (A.2) for $D = 3$ and $\xi_l = \alpha_{\tilde{q}_l}$. We can easily continue this recursive procedure to conjecture the formula (A.2) for odd D. To prove it, it is enough to show that the right-hand side of (A.2) satisfies the recursion relation (A.7). The right-hand side of (A.2) can be presented as $Y_{\mathcal{D}} = c_1 Y_{\mathcal{D}}^{(1)} + c_2 Y_{\mathcal{D}}^{(2)}$, where $c_1 = -(a+b)ab$, $c_2 = a+b$ and

$$Y_{\mathcal{D}}^{(1)} = c_D^{\mathrm{odd}}\frac{\prod_l (2r_l/a) f_l^{(D-1)/2} g_l^{(D-3)/2}}{\prod_{l<m}h_{l,m}}, \qquad Y_{\mathcal{D}}^{(2)} = Y_{\mathcal{D}}^{(1)}\prod_l \mathrm{e}^{\mathrm{i}\tilde{q}_l}. \tag{A.10}$$

Thus to prove (A.2), it suffices to prove that $Y_{\mathcal{D}}^{(1)}$ and $Y_{\mathcal{D}}^{(2)}$ satisfy (A.7).

Let us prove that $Y_{\mathcal{D}}^{(1)}$ satisfies the recurrence relation (A.7) with $\xi_l = \alpha_{\tilde{q}_l}$. Using the elementary relation $c_{D-2}^{\mathrm{odd}}/c_D^{\mathrm{odd}} = -\boldsymbol{\alpha}^{D-3}\boldsymbol{\beta}^{D-2}$ and (A.9), we reduce the problem to the proof of the identity

$$\begin{aligned} \frac{\prod_l (2r_l/a) f_l^{(D-1)/2} g_l^{(D-3)/2}}{\prod_{l<m}h_{l,m}} &= \sum_{k\neq s}\frac{\prod_{l\neq k,s}(2r_l/a) f_l^{(D-3)/2} g_l^{(D-5)/2}}{\prod_{l<m;l,m\neq k,s}h_{l,m}} \\ &\quad\times\frac{4r_k r_s}{a^2}\frac{f_s f_k^{D-2} g_k^{D-3}\mathrm{e}^{\mathrm{i}\tilde{q}_k}}{h_{s,k}}\prod_{l\neq k,s}\frac{f_l g_l}{h_{l,k}(\mathrm{e}^{\mathrm{i}\tilde{q}_l}-\mathrm{e}^{\mathrm{i}\tilde{q}_k})}. \end{aligned} \tag{A.11}$$

We see that all r_l and the $f_l, g_l, h_{l,m}$ with $l, m \neq k, s$ match between both sides of (A.11), leaving us with

$$\frac{(f_s g_s)^{(D-3)/2}}{\prod_{l\neq s}h_{l,s}} = \sum_{k\neq s}\frac{(f_k g_k)^{(D-3)/2}\,\mathrm{e}^{\mathrm{i}\tilde{q}_k}}{h_{k,s}\prod_{l\neq s,k}(\mathrm{e}^{\mathrm{i}\tilde{q}_l}-\mathrm{e}^{\mathrm{i}\tilde{q}_k})}, \tag{A.12}$$

which is equivalent to the interpolation identity (A.4) used here for the following choice of the parameters: $x_k = \mathrm{e}^{\mathrm{i}\tilde{q}_k}$ for $k \in \mathcal{D}/s$, $x_s = \mathrm{e}^{-\mathrm{i}\tilde{q}_s}$,

$$\{y_0, y_1, \ldots, y_{D-3}\} = \{0, \underbrace{a^2, \ldots, a^2}_{(D-3)/2\text{times}}, \underbrace{a^{-2}, \ldots, a^{-2}}_{(D-3)/2\text{times}}\}.$$

The proof that $Y_{\mathcal{D}}^{(2)}$ satisfies the recurrence relation (A.7) reduces to the same interpolation identity, but with y_0 omitted. This proves (A.2) for D odd and $\xi_l = \alpha_{\tilde{q}_l}$.

As was explained before, the change of the sign at ζ in (A.1) can be adjusted by changing the sign of b in the final formula. Similarly, the change of the sign at ξ_l can be adjusted by the simultaneous change of the signs of r_l and ζ. Finally, the transformation $b \to 1/b$ leads to $r_l \to r_l/b^2$, $-\alpha_{\tilde{q}_l} \to \beta_{\tilde{q}_l}/b^2$. This allows to find (A.1) at $\xi_l = \beta_{\tilde{q}_l}$ if we know (A.1) at $\xi_l = -\alpha_{\tilde{q}_l}$. The mentioned transformations cover all the cases of (A.1) for D odd.

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