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Spinons in magnetic chains of arbitrary spins at finite temperatures

J Suzuki†

Institute of Physics, University of Tokyo at Komaba, Komaba 3-8-1, Meguro-ku, Tokyo, Japan

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Abstract. The thermodynamics of solvable isotropic chains with arbitrary spins is addressed by the recently developed quantum transfer matrix (QTM) approach. The set of nonlinear equations which exactly characterizes the free energy is derived by respecting the physical excitations at $T = 0$, spinons and RSOS kinks. We argue the implication of the present formulation for a spinon character formula of the level-$k = 2S$ $SU(2)$ WZWN model.

1. Introduction

The 1D spin systems have been providing problems of both physical and mathematical interest. Among them, there exists a family of solvable models of Heisenberg type with spin-S [1, 2]. For instance, this includes,

$$\mathcal{H} = J \sum_{i=1}^{L} \{\vec{S}_i \vec{S}_{i+1} + \tfrac{1}{4}\} \tag{1}$$

$$\mathcal{H} = \frac{J}{4} \sum_{i=1}^{L} \{\vec{S}_i \vec{S}_{i+1} - (\vec{S}_i \vec{S}_{i+1})^2 + 3\} \tag{2}$$

as $S = \frac{1}{2}$, 1, respectively.

Ground state properties as well as low-lying excitations have been elucidated by the powerful machinery of solvable models, the Bethe ansatz equation (BAE). It has been demonstrated in many contexts [3–5] that the underlying field theory is the level-$k = 2S$ $SU(2)$ WZWN model [6].

Although this 1D quantum model is equivalent to a 2D vertex model, physical excitations have both the nature of vertex models and restricted SOS models. This was first demonstrated in [7] based on the S-matrix argument. The space of states is identified in [8]. Through the decomposition of crystals, these double features are made explicit in terms of 'type of domain walls' and 'type of domain'. There are independent justifications for this: the double feature in the spectral decomposition is shown by the path space approach [9]. See also [10] for the decomposition of the space picture realized in Fermionic forms.

Here we are interested in the finite-temperature problem. Standard arguments employ the string hypothesis [2, 11]. The excitation is described not in terms of 'physical excitations' in the above sense, but in the 'string basis'. There, strings of arbitrary lengths are allowed, which results in infinitely many coupled integral equations among infinitely many unknown

† E-mail address: suz@hep1.c.u-tokyo.ac.jp

functions. The description successfully reproduces the expected specific heat anomaly. It may not be, however, best suitable for practical numerics.

We revisit the problem via the recently developed commuting quantum transfer matrix (QTM) approach [13–20]. The formulation does not rely on the string hypothesis. Rather, it only relies on analyticity structures of the object called QTM [12, 21]. The problem of the combinatorial summation, i.e. evaluation of the partition function, then reduces to investigation of the analyticity of suitably chosen auxiliary functions. Up to now, two kinds of choices have been adopted independently:

(a) The eigenvalue of the QTM as given by the quantum inverse scattering method consists of several terms. The auxiliary functions are chosen from combinations of products of these terms [13–15, 17]. A convenient choice leads to a finite number of coupled nonlinear integral equations for a finite number of unknown functions.
(b) A set of auxiliary functions may be chosen from the fusion hierarchy among 'generalized' QTMs [12, 16, 18, 20]. Generically, one obtains an infinite number of coupled nonlinear integral equations for an infinite number of unknown functions. This can be shown to recover the conventional TBAs based on the string hypothesis. Of course, the new approach is entirely free of any assumption about excitations (unlike the string hypothesis).

The spin-1 case is analysed in the related problem, in the context of finite-size corrections [22, 23]. These six functions are introduced in the spirit of (*a*). The structure of NLIE among them is much more involved in comparison with the spin-$\frac{1}{2}$ case, and seems to defy a simple-minded generalization to higher S cases. In a sense the most subtle point in the QTM approach appears; one does not know an *a priori* 'better' set of auxiliary functions.

Here, we adopt another choice of auxiliary functions: in particular, for the spin-1 case the number of these functions is three in contrast to six as in [23]. A simple idea of combining the two formulations (*a*) and (*b*) works well so that the generalization to arbitrary S is possible. The adopted functions agree with the picture in [7]. Roughly speaking, the fusion part (*b*) of the auxiliary functions is related to the RSOS piece of the excitation, while auxiliary functions from (*a*) correspond to spinons.

We remark that the fusion hierarchy itself is not truncated, by brute force, into a finite set. Instead, the spinon part makes the functional relations among them strictly closed. Thus we obtain $2S + 1$ coupled integral equations for $2S + 1$ unknown functions.

Besides the practical advantage, this implies universality in the description of the thermodynamics of solvable quantum 1D chains, i.e. description only in terms of objects which reduce to physical excitations in $T \rightarrow 0$. This has already been demonstrated for several models in highly correlated 1D electron systems including the supersymmetric $t - J$ model [14], the supersymmetric extended Hubbard model [15] and the Hubbard model [17]. There the exact thermodynamics are formulated in terms of 'spinons' and 'holons', although they lose sense at sufficiently high temperatures. This paper adds one successful example even in the fusion models and gives further support to the above conjecture.

This paper is organized as follows. In section 2, we define the main object in this approach, the QTM. A minimal information of the novel approach is sketched. Section 3 is devoted to a brief description of the fusion hierarchy of generalized QTMs. After these preparations, we introduce auxiliary functions and examine functional relations among them in section 4. The analytic structure studied numerically leads to nonlinear integral equations as discussed in section 5. Based on these equations the low-temperature asymptotics are studied analytically in section 6. The central charge of the level-$k = 2S$ $SU(2)$ WZWN model is successfully recovered. We also present the numerical evaluation of the specific heat of $S = \frac{1}{2},\ 1,\ \frac{3}{2}$ models for wider ranges of temperatures. In section 7, the implication of the present formulation to

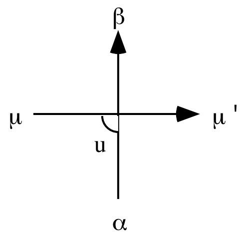

Figure 1. Graphical representation of the R-matrix (its element $\mathcal{R}_{\alpha\beta}^{\mu\mu'}$).

the spinon character formula of the WZWN model [9, 24, 42] is discussed. A summary of the paper is given in section 8.

2. QTM formulation

The present QTM formulation originates from two ingredients: the equivalence theorem between 1D quantum and 2D classical systems [21] on the one side and the integrability structure on the other [25]. The latter, in particular, provides a way of introducing commuting QTMs which reduce the problem of combinatorial counting to that of the analyticity of suitable auxiliary functions [12]. Such a strategy has been successfully applied to several interesting models [12–20]. We also mention earlier studies on thermodynamics [26–30] which essentially utilize only the former part of ideas.

A classical analogue to the solvable spin-S XXX model is already found as a $2S+1$ state vertex model [33]. The Boltzmann weights are identified with the matrix elements of the $\widehat{\mathfrak{sl}_2}$ invariant $R^\vee$ matrix:

$$
\begin{aligned}
R^\vee(u) &= \sum_{j=0}^{k} \rho_{2k-2j}(u) P_{2k-2j} \\
\rho_{2k-2j} &= \prod_{\ell=0}^{j-1} \frac{2(k-\ell)-u}{2(k-\ell)} \prod_{\ell=j}^{k-1} \frac{2(k-\ell)+u}{2(k-\ell)}
\end{aligned}
\tag{3}
$$

where $k = 2S$ and P_j is the projector to V_j, the $(j+1)$-dimensional irreducible module of sl_2. We choose $\{-j/2, -j/2+1, \ldots, j/2\}$ as basis for V_j. The spectral parameter u represents the anisotropy of the vertex weights. The Yang–Baxter equation implies the commutation of row-to-row transfer matrices for arbitrary spectral parameters u, v: $\mathcal{T}(u)\mathcal{T}(v) = \mathcal{T}(v)\mathcal{T}(u)$ with

$$
\mathcal{T}_\alpha^\beta(u) = \sum_\mu \prod_{i=1}^{L} \mathcal{R}_{\alpha_i\beta_i}^{\mu_i\mu_{i+1}}(u) \tag{4}
$$

where L denotes the real system size, $\alpha_i, \beta_i, \mu_i \in V_k$, $\mathcal{R} = PR^\vee$ and $P(x \otimes y) = y \otimes x$.

The Hamiltonian is obtained as the logarithmic derivative at $u = 0$,

$$
\mathcal{H} = J \frac{\mathrm{d}}{\mathrm{d}u} \ln \mathcal{T}(u)\Big|_{u=0}. \tag{5}
$$

It is an easy exercise to verify (5) gives (1) and (2) for $S = \frac{1}{2}, 1$ respectively. This may be done most easily by representing P_j in (3) by

$$
P_j = \prod_{p=0, p\neq j}^{k} \frac{\vec{S}\vec{S} - x_p}{x_j - x_p}
$$

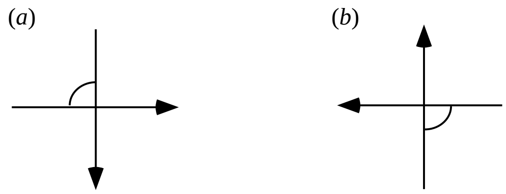

Figure 2. In the same spirit as figure 1, R-matrices, $\tilde{\mathcal{R}}$ (a) and $\bar{\mathcal{R}}$ (b) are depicted above.

and $x_j = \frac{1}{2}(\frac{j}{2}(\frac{j}{2}+1) - k(\frac{k}{2}+1))$. The Hamiltonian for general S can be extracted similarly. This is the well known expression of the equivalence between 1D quantum systems and 2D classical models. To utilize the equivalence in evaluating finite T quantities, in particular free energy, we need to proceed further.

Let us introduce Boltzmann weights $\tilde{\mathcal{R}}$ ($\bar{\mathcal{R}}$) of models related to (3) by clockwise (anticlockwise) 90° rotations:

$$\tilde{\mathcal{R}}^{\mu\nu}_{\alpha\beta}(v) = \mathcal{R}^{\beta\alpha}_{\mu\nu}(v) \qquad \bar{\mathcal{R}}^{\mu\nu}_{\alpha\beta}(v) = \mathcal{R}^{\alpha\beta}_{\nu\mu}(v).$$

The standard initial condition of the $R^{\vee}$-matrix and (5) lead to significant relations,

$$\mathcal{T}(u) = \mathcal{T}_R \mathrm{e}^{u\mathcal{H}/J+\mathcal{O}(u^2)} \qquad \bar{\mathcal{T}}(u) = \mathcal{T}_L \mathrm{e}^{u\mathcal{H}/J+\mathcal{O}(u^2)} \tag{6}$$

where $\bar{\mathcal{T}}$ is defined in analogy to (4), replacing $\mathcal{R}$ by $\bar{\mathcal{R}}$. $\mathcal{T}_{R,L}$ are the right- and left-shift operators, respectively, and they commute with the Hamiltonian.

We are ready to apply the Trotter formula; by substitution

$$u = -J\beta/N \tag{7}$$

we find

$$(\mathcal{T}(u)\bar{\mathcal{T}}(u))^{N/2} = \mathrm{e}^{-\beta\mathcal{H}+\mathcal{O}(1/N)}. \tag{8}$$

where β denotes the inverse temperature. N is a large integer 'Trotter' number, interpreted as a fictitious system size in a virtual direction. Thus, the partition function of the quantum system (size L, inverse temperature β)

$$Z = \lim_{N\to\infty} \mathrm{tr}(\mathcal{T}(u)\bar{\mathcal{T}}(u))^{N/2} \tag{9}$$

is identical to the partition function of an inhomogeneous $2S$+1 vertex model with alternating rows on a virtual 2D lattice of size $L \times N$ (see figure 3). Although the above mapping is exact, the expression (9) is not yet efficient. The eigenvalues of $\mathcal{T}(u)\bar{\mathcal{T}}(u)$ are almost degenerate. Hence it is still a difficult task to evaluate the trace. The intriguing point in [21] is to consider a transfer matrix $\tilde{\mathcal{T}}(u)$ propagating in the 'horizontal' direction.

This novel operator acting on N sites, has gaps in the eigenvalues provided $T > 0$. Here we adopt the more sophisticated approach developed in [12–20]. Explicitly, we define the QTM by

$$\mathcal{T}_{\mathrm{QTM}}(u,x) = \sum_{\mu} \prod_{i=1}^{N/2} \mathcal{R}^{\mu_{2i-1}\mu_{2i}}_{\alpha_{2i-1}\beta_{2i-1}}(u+\mathrm{i}x)\tilde{\mathcal{R}}^{\mu_{2i}\mu_{2i+1}}_{\alpha_{2i}\ \beta_{2i}}(u-\mathrm{i}x) \tag{10}$$

which reduces to above-mentioned $\tilde{\mathcal{T}}(u)$ by putting $x = 0$. Figure represents the QTM graphically. Though the introduction of the extra parameter x seems to be redundant, there is a remarkable property:

$$[\mathcal{T}_{\mathrm{QTM}}(u,x), \mathcal{T}_{\mathrm{QTM}}(u,x')] = 0 \tag{11}$$

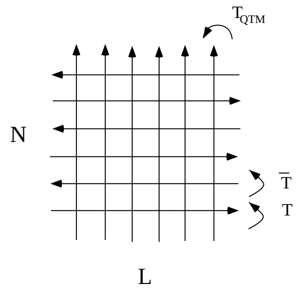

Figure 3. Graphic representation of the partition function on a virtual two-dimensional lattice of $N \times L$. The operators $\mathcal{T}, \bar{\mathcal{T}}$ transfer states from bottom to top, while $\tilde{\mathcal{T}}(u)$ and $\mathcal{T}_{\mathrm{QTM}}$ do so from right to left.

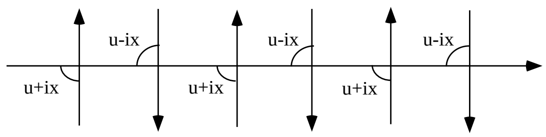

Figure 4. Graphic representation of $\mathcal{T}_{\mathrm{QTM}}(u, v)$.

by fixing u. This originates from the fact that $\mathcal{R}$ and $\tilde{\mathcal{R}}$ operators possess the same intertwiner. Thus for each T, one can associate an auxiliary complex plane x to the partition function.

Due to the gap in spectra, the free energy f of 1D quantum spin chains is given only by the largest eigenvalue $\Lambda_{\mathrm{QTM}}(u, x)$,

$$f = -\frac{1}{\beta} \lim_{L\to\infty} \frac{1}{L} \ln Z = -\frac{1}{\beta} \lim_{N\to\infty} \ln \Lambda_{\mathrm{QTM}} \left(u = \frac{-\beta J}{N}, x = 0 \right). \tag{12}$$

This is the starting point of our analysis. The difficulty in evaluating (12) lies in the N dependence of the vertex weights. The numerical extrapolation through finite N studies may be plagued by marginal perturbations [19]. The prescription is to utilize the existence of the complex plane x for each T. The analytic properties of $\mathcal{T}_{\mathrm{QTM}}$ and suitably chosen auxiliary functions in the x-plane make the evaluation possible and transparent.

Before closing this section, we shall describe how to modify the above relations in the presence of an external magnetic field H, namely by inclusion of the Zeeman term $-2H \sum_i S_i^z$ to the Hamiltonian (5). This contribution is described by diagonal operator $D(H)$,

$$\begin{pmatrix} \mathrm{e}^{-2S\beta H} \\ \mathrm{e}^{-(2S-1)\beta H} \\ \vdots \\ \mathrm{e}^{2S\beta H} \end{pmatrix} \otimes \begin{pmatrix} \mathrm{e}^{-2S\beta H} \\ \mathrm{e}^{-(2S-1)\beta H} \\ \vdots \\ \mathrm{e}^{2S\beta H} \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} \mathrm{e}^{-2S\beta H} \\ \mathrm{e}^{-(2S-1)\beta H} \\ \vdots \\ \mathrm{e}^{2S\beta H} \end{pmatrix}.$$

Thus, one has only to insert this inside the trace (9):

$$Z = \lim_{N\to\infty} \mathrm{tr}(\mathcal{T}(u)\bar{\mathcal{T}}(u))^{N/2} D(H).$$

In the rotated frame, the effect of the insertion of $D(H)$ is translated to the boundary weight, $B(\mu_1) = \mathrm{e}^{\beta\mu_1 H}$;

$$\mathcal{T}_{\mathrm{QTM}}(u, x) = \sum_{\mu} B(\mu_1) \prod_{i=1}^{N/2} \mathcal{R}^{\mu_{2i-1}\,\mu_{2i}}_{\alpha_{2i-1}\,\beta_{2i-1}}(u + \mathrm{i}x)\, \tilde{\mathcal{R}}^{\mu_{2i}\,\mu_{2i+1}}_{\alpha_{2i}\,\beta_{2i}}(u - \mathrm{i}x).$$

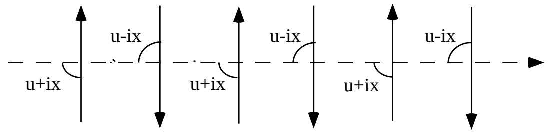

Figure 5. For $T_j(u,x)$, the vertical arrows carry V_k while the horizontal (broken) arrow carries V_j.

3. Fusion hierarchy

We consider a hierarchy of quantum transfer matrices acting on $V_k^{\otimes N}$. Let $T_j(u,x)$ be a member of the hierarchy with the auxiliary space V_j.

In other words, it is the transfer matrix of the vertex model of which spins $S(=k/2)$ are assigned to vertical edges and spins $j/2$ to horizontal edges (figure 5). The quantity of our interest, $T_{\mathrm{QTM}}(u,x)$ coincides with $T_k(u,x)$ apart from over-all normalization, which is specified later.

For brevity, we shall only give matrix elements of $\mathcal{R}(u)$ defining the most fundamental $T_1(u,x)$.

$$\mathcal{R}_{\ell,\ell}^{\pm1/2,\pm1/2}(u) = u+1\pm2\ell \qquad \mathcal{R}_{\ell',\ell}^{\ell'-\ell,\ell-\ell'}(u) = \sqrt{(k+2+2\min(\ell,\ell'))(k-2\min(\ell,\ell'))}$$

where $\ell,\ell' \in \{-k/2\ldots,k/2\}$ and $|\ell-\ell'|=1$. Similar to (3), the corresponding $R^\vee$ matrix has decomposition:

$$R^\vee(u) = (u+k+1)P_{k+1} + (u-k-1)P_{k-1}. \tag{13}$$

The $\mathcal{R}$-matrix for $T_j(u,x)$ is obtained from the above elementary $\mathcal{R}(u)$ by $j-1$ times fusion in the auxiliary space. By the construction, arbitrary pairs in this hierarchy are commutative if they share the same u:

$$[T_j(u,x), T_{j'}(u,x')] = 0.$$

This is a generalization of (11). In the following, we fix u for all QTMs and omit the dependency on u. Due to the consequential commutativity, one needs not distinguish operators T_j from their eigenvalues.

Then the explicit eigenvalue of the most elementary transfer matrix $T_1(x)$ reads

$$\begin{aligned} T_1(x) &= \phi_+(x-(k-1)\mathrm{i})\phi_-(x-(k+1)\mathrm{i})\mathrm{e}^{\beta H}\frac{Q(x+2\mathrm{i})}{Q(x)} \\ &\quad+\phi_-(x+(k-1)\mathrm{i})\phi_+(x+(k+1)\mathrm{i})\mathrm{e}^{-\beta H}\frac{Q(x-2\mathrm{i})}{Q(x)} \\ \phi_\pm(x) &:= (x\pm \mathrm{i}u)^{N/2} \\ Q(x) &:= \prod_{j=1}^{m}(x-x_j) \end{aligned} \tag{14}$$

where x_j, $(j=1,\ldots,m)$ denotes the solution to the Bethe ansatz equation:

$$\frac{\phi_-(x_j+(k-1)\mathrm{i})\phi_+(x_j+(k+1)\mathrm{i})}{\phi_+(x_j-(k-1)\mathrm{i})\phi_-(x_j-(k+1)\mathrm{i})} = -\mathrm{e}^{2\beta H}\frac{Q(x_j+2\mathrm{i})}{Q(x_j-2\mathrm{i})}.$$

The number of BAE roots, m, differs for different eigenstates generally, and $m = Nk/2$ for the largest eigenvalue case.

By construction of the fusion hierarchy and from singularities of the intertwining operators (13) by tentatively replacing $k\to j$, the following relation is valid:

$$T_j(x)T_1(x-\mathrm{i}(j+1)) = T_{j+1}(x-\mathrm{i}) + g_j(x)T_{j-1}(x+\mathrm{i})$$

$$g_j(x) = \phi_-(x-\mathrm{i}(k+j+2))\phi_-(x+\mathrm{i}(k-j))\phi_+(x-\mathrm{i}(j+k))\phi_+(x+\mathrm{i}(k-j+2)).$$

From this, one can prove the important functional relation (T-system) by induction [36],

$$
\begin{aligned}
&T_p(x+\mathrm{i})T_p(x-\mathrm{i}) = f_p(x) + T_{p-1}(x)T_{p+1}(x) \qquad (p \geqslant 1)\\
&f_p(x) := \prod_{j=1}^{p}\prod_{\sigma=\pm} \phi_\sigma(x+\mathrm{i}\sigma(p-k-2j+1))\phi_\sigma(x+\mathrm{i}\sigma(k-p+2j+1))
\end{aligned}
\tag{15}
$$

and $T_0 = 1$.

By substituting (14) into (15), we can successively obtain $T_p(x), (p \geqslant 2)$. Explicitly, $T_p(x)$ consists of a sum of $p+1$ terms,

$$
\begin{aligned}
T_p(x) &:= \sum_{\ell=1}^{p+1} \lambda_\ell^{(p)}(x)\\
\lambda_\ell^{(p)}(x) &:= \mathrm{e}^{\beta H(p+2-2\ell)} \psi_\ell^{(p)}(x) \frac{Q(x+\mathrm{i}(p+1))Q(x-\mathrm{i}(p+1))}{Q(x+\mathrm{i}(2\ell-p-1))Q(x+\mathrm{i}(2\ell-p-3))}\\
\psi_\ell^{(p)}(x) &:= \prod_{j=1}^{p-\ell+1} \phi_-(x+\mathrm{i}(p-k-2j))\phi_+(x+\mathrm{i}(p-k+2-2j))\\
&\quad\times \prod_{j=1}^{\ell-1} \phi_-(x-\mathrm{i}(p-k+2-2j))\phi_+(x-\mathrm{i}(p-k-2j)).
\end{aligned}
\tag{16}
$$

As has been noted, $T_k(x)$ has a normalization trivially different from $T_{\mathrm{QTM}}(u,x)$ in the previous section:

$$
\begin{aligned}
T_{\mathrm{QTM}}(u,x) &= \frac{T_k(x)}{\prod_{p=1}^{k}\phi_0(2\mathrm{i}p)}\\
\phi_0(x) &:= x^{N/2}.
\end{aligned}
\tag{17}
$$

In the original problem of the spin-S chain, only $T_k(x)$ is of interest. The auxiliary T_j, however, make the evaluation of $T_k(x)$ transparent, as is shown in the following.

4. Auxiliary functions and functional relations among them

To explore the analyticity of the transfer matrix $T_k(x)$, we introduce $k+1$ auxiliary functions. The first $k-1$ functions $\{y_j(x)\}$ have been used in many works and have a sound basis in the sl_2 fusion hierarchy. They are defined by [36,37]

$$
y_j(x) := \frac{T_{j-1}(x)T_{j+1}(x)}{f_j(x)} \qquad j \geqslant 1.
$$

The functional relations among them are sometimes referred to as the Y-system:

$$
\begin{aligned}
y_j(x+\mathrm{i})y_j(x-\mathrm{i}) &= Y_{j-1}(x)Y_{j+1}(x) \qquad j \geqslant 1\\
Y_j(x) &:= 1 + y_j(x)
\end{aligned}
\tag{18}
$$

and $y_0(x) := 0$ which is a consequence of equation (15). Note that the Y-system is not truncated to a finite set in this case. The $(k-1)$th equation, which characterizes $y_{k-1}(x)$, inevitably contains $y_k(x)$ in the rhs, and so on. Thus, another device is needed to construct a finite set of auxiliary functions satisfying a complete and closed set of functional relations. The remaining two functions $\mathfrak{b}(x)$, $\bar{\mathfrak{b}}(x)$ and their 'relatives' $\mathfrak{B}(x) := 1 + \mathfrak{b}(x)$, $\bar{\mathfrak{B}}(x) := 1 + \bar{\mathfrak{b}}(x)$ play this role. We define them by ratios of λ in $T_k(x)$ as,

$$
\begin{aligned}
\mathfrak{b}(x) &:= \frac{\lambda_1^{(k)}(x+\mathrm{i}) + \cdots + \lambda_k^{(k)}(x+\mathrm{i})}{\lambda_{k+1}^{(k)}(x+\mathrm{i})}\\
\bar{\mathfrak{b}}(x) &:= \frac{\lambda_2^{(k)}(x-\mathrm{i}) + \cdots + \lambda_{k+1}^{(k)}(x-\mathrm{i})}{\lambda_1^{(k)}(x-\mathrm{i})}.
\end{aligned}
\tag{19}
$$

The following relations are direct consequences of the above definitions:

$$\begin{aligned}
\mathfrak{B}(x)\lambda^{(k)}_{k+1}(x+\mathrm{i}) &= \mathrm{e}^{-k\beta H}\mathfrak{B}(x)\prod_{\sigma=\pm}\prod_{j=1}^{k}\phi_\sigma(x+(2j+\sigma)\mathrm{i})\frac{Q(x-\mathrm{i}k)}{Q(x+\mathrm{i}k)} = T_k(x+\mathrm{i}) \\
\bar{\mathfrak{B}}(x)\lambda^{(k)}_{1}(x-\mathrm{i}) &= \mathrm{e}^{k\beta H}\bar{\mathfrak{B}}(x)\prod_{\sigma=\pm}\prod_{j=1}^{k}\phi_\sigma(x-(2j-\sigma)\mathrm{i})\frac{Q(x+\mathrm{i}k)}{Q(x-\mathrm{i}k)} = T_k(x-\mathrm{i}).
\end{aligned} \tag{20}$$

We have $k-1$ equations for y_j, $(j=1,\ldots,k-1)$ in terms of $Y_j(x)$, $(j=1,\ldots,k-1)$, $\mathfrak{B}(x)$ and $\bar{\mathfrak{B}}(x)$. The first $k-2$ equations are chosen directly from the Y-system. In the $(k-1)$th equation, we rewrite $Y_k(x)$ in the rhs of the Y-system ($j=k-1$ in (18)) by $\mathfrak{B}(x)\bar{\mathfrak{B}}(x)$, thanks to (20), the definitions of y_k, Y_k and the functional relation (15):

$$y_{k-1}(x-\mathrm{i})y_{k-1}(x+\mathrm{i}) = Y_{k-2}(x)\mathfrak{B}(x)\bar{\mathfrak{B}}(x). \tag{21}$$

Finally, equations for $\mathfrak{b}$ in terms of $Y_j(x)$, $(j=1,\ldots,k-1)$, $\mathfrak{B}(x)$ and $\bar{\mathfrak{B}}(x)$ are to be found. By comparing explicit forms, one finds

$$\begin{aligned}
\mathfrak{b}(x) &= \mathrm{e}^{\beta(k+1)H}\prod_{\sigma=\pm}\frac{\phi_\sigma(x+\mathrm{i}\sigma)}{\prod_{j=1}^{k}\phi_\sigma(x+(2j+\sigma)\mathrm{i})}\frac{Q(x+\mathrm{i}(k+2))}{Q(x-\mathrm{i}k)}T_{k-1}(x) \\
\bar{\mathfrak{b}}(x) &= \mathrm{e}^{-\beta(k+1)H}\prod_{\sigma=\pm}\frac{\phi_\sigma(x+\mathrm{i}\sigma)}{\prod_{j=1}^{k}\phi_\sigma(x-(2j-\sigma)\mathrm{i})}\frac{Q(x-\mathrm{i}(k+2))}{Q(x+\mathrm{i}k)}T_{k-1}(x).
\end{aligned} \tag{22}$$

Note that $T_{k-1}(x)$ is presented by $Y_{k-1}(x)$:

$$T_{k-1}(x-\mathrm{i})T_{k-1}(x+\mathrm{i}) = f_{k-1}(x)Y_{k-1}(x) \tag{23}$$

which originates directly from definitions of y_{k-1}, Y_{k-1} and the functional relation (15).

In what follows, we analyse these functional relations via the Fourier transformation. One denotes $\widehat{dl}\mathfrak{b}[q]$ to mean the Fourier transformation of the logarithmic derivative of $\mathfrak{b}(x)$:

$$\widehat{dl}\mathfrak{b}[q] := \int_{-\infty}^{\infty}\frac{\mathrm{d}\log\mathfrak{b}(x)}{\mathrm{d}x}\mathrm{e}^{\mathrm{i}qx}\,\mathrm{d}x$$

and similarly for other functions. With some assumptions of the analytic properties of the auxiliary functions, the above functional relations can be transformed into algebraic equations in the Fourier space. Roughly speaking, one can solve $\widehat{dl}Q[q]$ functions in terms of $\widehat{dl}\mathfrak{B}[q]$ and $\widehat{dl}\bar{\mathfrak{B}}[q]$ by deleting $\widehat{dl}T_k[q]$ from algebraic equations originated from (20). Similarly $\widehat{dl}T_{k-1}[q]$ is solved by $\widehat{dl}Y_{k-1}[q]$ from (23). Substituting these results into Fourier transformations of logarithmic derivatives of (22), one finds expressions of $\widehat{dl}\mathfrak{b}[q]$, $\widehat{dl}\bar{\mathfrak{b}}[q]$ in terms of $\widehat{dl}\mathfrak{B}[q]$, $\widehat{dl}\bar{\mathfrak{B}}[q]$ and $\widehat{dl}Y_{k-1}[q]$. After inverse-Fourier transformation and integration over x, one obtains the desired finite set of equations. We will make the above-mentioned analytic assumptions explicit and examine them in the next section.

Before going into details, let us discuss the physical interpretation of the above functions. As is argued in [7], the S-matrix of excitations in the spin-S model factorizes into two pieces: the spin-$\frac{1}{2}$ $SU(2)$ S-matrix and the RSOS S-matrix of sl_2 level-$k=2S$. This is consistent with the general expectation that the underlying field theory is the level-k $SU(2)$ WZWN model. The latter is known to 'decompose' into Gaussian and Z_k parafermionic field theories [34]. One finds, see for instance [35], evidence for the equivalence between the sl_2 RSOS model in regime II and the Z_k parafermion field theory in the scaling limit. In the present description, $\mathfrak{b}$, $\bar{\mathfrak{b}}$ are to be identified with up- and down-spinons. As we will see later, only they couple to the magnetic field directly. For the $S=\frac{1}{2}$ case, there is further direct evidence for this identification [51]. On the other hand, $\{y_j(x)\}$ are insensitive to the external field. We are led to identify $y_j(x)$ in our choice as the RSOS piece of the excitations. The RSOS model possesses a subset of the Y-system (18). The additional condition $y_k = 0$ for the model leads to the truncated set of equations among $k-1$ y [36, 38]. In the present problem, at sufficiently low temperatures, one observes, $|\mathfrak{b}|, |\bar{\mathfrak{b}}| \sim 0$ for $x << \ln\beta$. Thus the substitution of $\mathfrak{B} = \bar{\mathfrak{B}} = 1$ in (21) might be legitimate in the vicinity of the origin. Then the resultant approximated Y-system coincides with that of the RSOS model. In this sense, (21) represents a gluing relation between spinon and RSOS parts of excitations.

5. Nonlinear integral equations

We derive the nonlinear integral equations among auxiliary functions introduced in the previous section. The crucial observation is, that all nontrivial zeros and singularities of these functions are determined by zeros of $Q(x)$ and $T_j(x)$, $(j = 1, \ldots, k)$. For the largest eigenvalue sector of $T_k(x)$, zeros of $Q(x)$ form so-called k-strings. Imaginary parts of zeros are approximately located at $(k+1) - 2\ell$, $\ell = 1, \ldots, k$. For later use, we introduce the notations,

$$\Psi_1(x) := Q(x - \mathrm{i}k) \qquad \Psi_2(x) := Q(x + \mathrm{i}k). \tag{24}$$

Empirically, similar patterns are found for zeros of $T_j(x)$: they distribute approximately on lines, $\mathrm{Im}\, x = \pm(k + j - 2\ell), \ell = 0, \ldots, j-1$. We assume that these observation from numerics with fixed N is valid and that the deviations from lines are very small in the limit $N \to \infty$. Then one deduces the following ansatz on the strips where auxiliary functions are analytic, nonzero and have constant asymptotic behaviour (ANZC):

$$\begin{array}{ll}
\mathfrak{b}(x), \mathfrak{B}(x) & -1 < \mathrm{Im}\, x \leqslant 0 \\
\bar{\mathfrak{b}}(x), \bar{\mathfrak{B}}(x) & 0 \leqslant \mathrm{Im}\, x < 1 \\
y_j(x), Y_j(x) (j = 1, \ldots, k-1) \quad T_p(x), (p = 1, \ldots, k) & -1 \leqslant \mathrm{Im}\, x \leqslant 1 \\
\Psi_1(x) & \mathrm{Im}\, x < 0 \\
\Psi_2(x) & \mathrm{Im}\, x > 0.
\end{array}$$

We find it convenient to shift the definition of the arguments in $\mathfrak{b}, \mathfrak{B}, \bar{\mathfrak{b}}$ and $\bar{\mathfrak{B}}$. To avoid confusion, these new functions are denoted as $\mathfrak{a}$ etc,

$$\mathfrak{a}(x) := \mathfrak{b}(x - \mathrm{i}\gamma) \qquad \bar{\mathfrak{a}}(x) := \bar{\mathfrak{b}}(x + \mathrm{i}\gamma)$$

and similarly for capital functions. Here $0 < \gamma < \frac{1}{2}$ is an arbitrary but fixed parameter. Note that this is equivalent to adopt small shifts in the definition of the integration contours for the Fourier transformation. Due to the ANZC properties of $\mathfrak{b}, \bar{\mathfrak{b}}$, such modifications are almost trivial in the Fourier space.

Having identified ANZC strips, we revisit equations (20). Consider the integral,

$$\int_{\mathcal{C}} \frac{\mathrm{d}}{\mathrm{d}z} \log T_k(z) \mathrm{e}^{\mathrm{i}qz}\, \mathrm{d}z$$

where $\mathcal{C}$ encircles the edges of 'square': $[-\infty - \mathrm{i}, \infty - \mathrm{i}] \cup [\infty - \mathrm{i}, \infty + \mathrm{i}] \cup [\infty + \mathrm{i}, -\infty + \mathrm{i}] \cup [-\infty + \mathrm{i}, -\infty - \mathrm{i}]$ in counterclockwise manner. Due to the ANZC property of $\frac{\mathrm{d}}{\mathrm{d}z} \log T_k(z)$ inside $\mathcal{C}$, the following equation is valid from Cauchy's theorem:

$$0 = \int_{-\infty}^{\infty} \frac{\mathrm{d}}{\mathrm{d}x} \log T_k(x - \mathrm{i}) \mathrm{e}^{\mathrm{i}q(x-\mathrm{i})}\, \mathrm{d}x - \int_{-\infty}^{\infty} \frac{\mathrm{d}}{\mathrm{d}x} \log T_k(x + \mathrm{i}) \mathrm{e}^{\mathrm{i}q(x+\mathrm{i})}\, \mathrm{d}x.$$

One substitutes equations (20), rewritten in terms of $\Psi_{1,2}(x), \mathfrak{A}(x), \bar{\mathfrak{A}}(x)$, into the above equation and derives identities among $\widehat{dl}\Psi_{1,2}[q], \widehat{dl}\mathfrak{A}[q], \widehat{dl}\bar{\mathfrak{A}}[q]$,

$$\widehat{dl}\Psi_1[q < 0] = 0$$

$$\widehat{dl}\Psi_1[q > 0] = \frac{\mathrm{e}^{(1-\gamma)q}}{2\cosh q} \widehat{dl}\bar{\mathfrak{A}}[q] - \frac{\mathrm{e}^{-(1-\gamma)q}}{2\cosh q} \widehat{dl}\mathfrak{A}[q] + \pi \mathrm{i} N \frac{\mathrm{e}^{-kq} \sinh kq \cosh(1+u)q}{\cosh q \sinh q}$$

$$\widehat{dl}\Psi_2[q < 0] = -\frac{\mathrm{e}^{(1-\gamma)q}}{2\cosh q}\widehat{dl}\bar{\mathfrak{A}}[q] + \frac{\mathrm{e}^{-(1-\gamma)q}}{2\cosh q}\widehat{dl}\mathfrak{A}[q] - \pi\mathrm{i}N\frac{\mathrm{e}^{kq}\sinh kq\cosh(1+u)q}{\cosh q\sinh q}$$
$$\widehat{dl}\Psi_2[q > 0] = 0$$

and $\widehat{dl}\Psi_1[q = 0] = -\widehat{dl}\Psi_2[q = 0] = \pi Nk\mathrm{i}$. Similarly, one can derive an identity for $\widehat{dl}y_j[q]$ and $\widehat{dl}Y_j[q]$ from (18), and $\widehat{dl}T_{k-1}[q]$ and $\widehat{dl}Y_{k-1}[q]$ from (23). Substituting these relations into the original definitions of $\mathfrak{a}$ and $\bar{\mathfrak{a}}$, we obtain $k+1$ algebraic relations in Fourier space. (Remember $\Psi_{1,2}(x)$ are related to $Q(x)$ by (24).) After taking the inverse Fourier transformation and integrating over x once, we arrive at the $k+1$ coupled nonlinear integral equations:

$$\begin{pmatrix} \log y_1(x) \\ \vdots \\ \log y_{k-1}(x) \\ \log \mathfrak{a}(x) \\ \log \bar{\mathfrak{a}}(x) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \beta H + d(u, x - \mathrm{i}\gamma) \\ -\beta H + d(u, x + \mathrm{i}\gamma) \end{pmatrix} + \mathcal{K} * \begin{pmatrix} \log Y_1(x) \\ \vdots \\ \log Y_{k-1}(x) \\ \log \mathfrak{A}(x) \\ \log \bar{\mathfrak{A}}(x) \end{pmatrix} \tag{25}$$

where $(\mathcal{K} * g)_i$ denotes the matrix convolution $\sum_j \int \mathcal{K}_{i,j}(x-y)(g(y))_j\,\mathrm{d}y$ and the 'driving' function $d(u, x)$ reads

$$d(u, x) = \frac{N}{2}\int \frac{\sinh uq}{q\cosh q}\mathrm{e}^{-\mathrm{i}qx}\,\mathrm{d}q.$$

The integration constants ($\pm\beta H$) are fixed by comparing asymptotic values ($|x| \to \infty$) of both sides.

Explicitly the kernel matrix is given by

$$\mathcal{K}(x) := \begin{pmatrix} 0 & K(x) & 0 & \cdots & 0 & 0 & 0 & 0 \\ K(x) & 0 & K(x) & \cdots & 0 & 0 & & \\ 0 & K(x) & & & 0 & 0 & \vdots & \vdots \\ \vdots & & & & \vdots & \vdots & & \\ 0 & & \cdots & & 0 & K(x) & 0 & 0 \\ 0 & & & & K(x) & 0 & K(x+\mathrm{i}\gamma) & K(x-\mathrm{i}\gamma) \\ 0 & & \cdots & & 0 & K(x-\mathrm{i}\gamma) & F(x) & -F(x+2\mathrm{i}(1-\gamma)) \\ 0 & & \cdots & & 0 & K(x+\mathrm{i}\gamma) & -F(x-2\mathrm{i}(1-\gamma)) & F(x) \end{pmatrix} \tag{26}$$

where

$$K(x) := \frac{1}{4\cosh\pi x/2}$$
$$F(x) := \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-|q|-\mathrm{i}qx}}{2\cosh q}\,\mathrm{d}q.$$

T_k, in terms of these auxiliary functions, can be derived similarly. Technically, we find it convenient to introduce

$$T_k^R(x) := \frac{T_k(x)}{\prod_{p=1}^{k}\phi_{e(p)}(x - 2\mathrm{i}(k+1-p))\phi_{e(p+1)}(x + 2\mathrm{i}(k+1-p))} \tag{27}$$

and $e(p) = +(-)$ for $p =$ even (odd). Then the product of two equations in (20) leads to a simple algebraic relation:

$$T_k^R(x-\mathrm{i})T_k^R(x+\mathrm{i}) = \begin{cases} \mathfrak{B}(x)\bar{\mathfrak{B}}(x) & \text{for } k \text{ even} \\ \mathfrak{B}(x)\bar{\mathfrak{B}}(x)\dfrac{\phi_-(x+\mathrm{i})\phi_+(x-\mathrm{i})}{\phi_-(x-\mathrm{i})\phi_+(x+\mathrm{i})} & \text{for } k \text{ odd.} \end{cases} \tag{28}$$

From the ANZC property of both sides of (28) in appropriate strips, the logarithmic derivative of them reduces to a simple algebraic equation in Fourier space. Taking account of the normalization (17) and (27), we have

$$\log \Lambda_{QTM}(u,x) = \log \Lambda^{(0)}_{QTM}(u,x) + \int \frac{\log \mathfrak{A}(y)}{4\cosh \pi/2(x-y+\mathrm{i}\gamma)}\,\mathrm{d}y + \int \frac{\log \bar{\mathfrak{A}}(y)}{4\cosh \pi/2(x-y-\mathrm{i}\gamma)}\,\mathrm{d}y \tag{29}$$

$$\log \Lambda^{(0)}_{QTM}(u,x) := -\delta_{k=1(\mathrm{mod}2)}\frac{N}{2}\int \mathrm{e}^{-\mathrm{i}qx-|q|}\frac{\sinh uq}{q\cosh q}\,\mathrm{d}q + \sum_{p=1}^{k}\log\left\{\frac{\phi_{e(p)}(x-2\mathrm{i}(k+1-p))\phi_{e(p+1)}(x+2\mathrm{i}(k+1-p))}{\phi_0(2\mathrm{i}p)^2}\right\}. \tag{30}$$

Finally put $u = -\beta J/N$ and send $N \to \infty$ *analytically*. This merely amounts to replacements:

$$\begin{aligned} d(u,x) &\to D(x) = -\frac{\beta J\pi}{2\cosh \pi/2x} \\ \log \Lambda^{(0)}_{QTM}(u,x=0) &\to -\beta e_0 = -\frac{\beta J}{2}\sum_{j=1}^{k}\frac{(-1)^{k-j}}{j} + \delta_{k=1(\mathrm{mod}2)}\beta J\log 2. \end{aligned} \tag{31}$$

Note that e_0 coincides with the known ground state energy [2] after a trivial shift which stems from the difference in the normalization of $R^\vee$. The $k+1$ coupled nonlinear integral equations and $\log \Lambda_{QTM}$ do not carry the fictitious parameter N any longer. They efficiently describe the thermodynamics of the solvable spin-S XXX model. For an illustration, the specific heat for $S = \frac{1}{2},\ 1,\ \frac{3}{2}$ is evaluated for a wide range of temperature and plotted in figure 6. Each curve is produced by a 10–30 min CPU time calculation on a Micro Sparc work station. In the next section, we derive the low-temperature properties using (25), (30) and (31).

6. Analytic evaluation of the low-temperature asymptotics

We consider $T \to 0$ for the vanishing magnetic field. In a sufficiently low-temperature regime, $\mathfrak{a}, \log \mathfrak{A}$ shows a sharp crossover behaviour like a step function: $|\mathfrak{a}|, |\log \mathfrak{A}| \ll 1$ for $|x| < \frac{2}{\pi}\log \pi\beta J$ and $|\mathfrak{a}|, |\log \mathfrak{A}| = \mathrm{O}(1)$ for $|x| > \frac{2}{\pi}\log \pi\beta J$. Thus the following scaling functions [23] control the asymptotic behaviour:

$$\begin{aligned} la^{\pm}(\xi) &:= \log \mathfrak{a}\left(\pm\frac{2}{\pi}(\xi+\log \pi\beta J)\right) & lA^{\pm}(\xi) &:= \log \mathfrak{A}\left(\pm\frac{2}{\pi}(\xi+\log \pi\beta J)\right) \\ l\bar{a}^{\pm}(\xi) &:= \log \bar{\mathfrak{a}}\left(\pm\frac{2}{\pi}(\xi+\log \pi\beta J)\right) & l\bar{A}^{\pm}(\xi) &:= \log \bar{\mathfrak{A}}\left(\pm\frac{2}{\pi}(\xi+\log \pi\beta J)\right) \\ ly_p^{\pm}(\xi) &:= \log y_p\left(\pm\frac{2}{\pi}(\xi+\log \pi\beta J)\right) & lY_p^{\pm}(\xi) &:= \log Y_p\left(\pm\frac{2}{\pi}(\xi+\log \pi\beta J)\right). \end{aligned} \tag{32}$$

In terms of these scaling functions, NLIE are expressed by,

$$\begin{aligned} \begin{pmatrix} ly_1^{\pm}(\xi) \\ \vdots \\ ly_{k-1}^{\pm}(\xi) \\ la^{\pm}(\xi) \\ l\bar{a}^{\pm}(\xi) \end{pmatrix} &= \begin{pmatrix} 0 \\ \vdots \\ 0 \\ -\mathrm{e}^{-\xi\pm\mathrm{i}\gamma\pi/2} \\ -\mathrm{e}^{-\xi\mp\mathrm{i}\gamma\pi/2} \end{pmatrix} + \bar{\mathcal{K}} * \begin{pmatrix} lY_1^{\pm}(\xi) \\ \vdots \\ lY_{k-1}^{\pm}(\xi) \\ lA^{\pm}(\xi) \\ l\bar{A}^{\pm}(\xi) \end{pmatrix} \\ \bar{\mathcal{K}}(\xi) &= \frac{2}{\pi}\mathcal{K}\left(\frac{2\xi}{\pi}\right). \end{aligned} \tag{33}$$

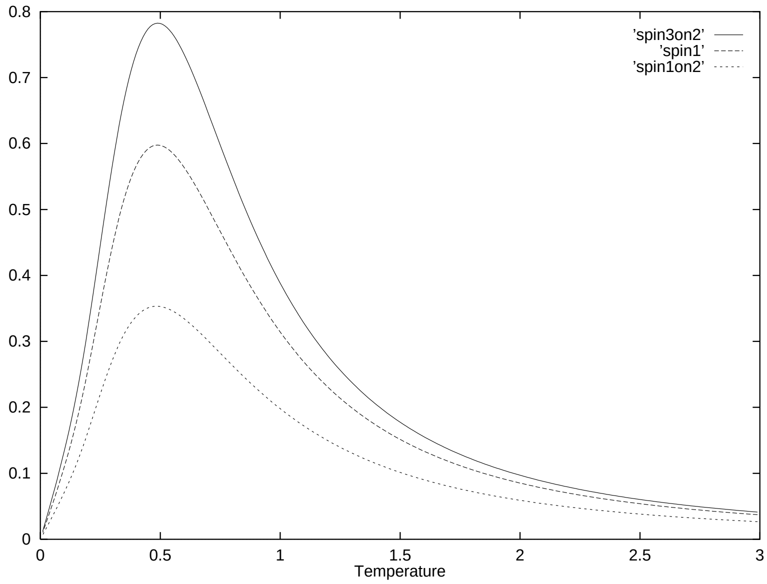

Figure 6. Specific heats for $S = \frac{3}{2}$, 1 and $\frac{1}{2}$ from top to bottom.

Note that neglect of small corrections $\sim \mathrm{O}(T)$ leads to the decoupling equations for $\pm$.

The thermal contribution (the second and the third term in (30)) to $\lim_{N\to\infty} \log \Lambda_{\mathrm{QTM}}(u = -\frac{\beta J}{N}, x)$ reads,

$$\begin{aligned}&\frac{\mathrm{e}^{\pi x/2}}{\pi^2 \beta J}\left[\mathrm{e}^{\mathrm{i}\gamma\pi/2}\int \mathrm{e}^{-\xi} lA^{+}\,\mathrm{d}\xi + \mathrm{e}^{-\mathrm{i}\gamma\pi/2}\int \mathrm{e}^{-\xi} l\bar{A}^{+}\,\mathrm{d}\xi\right] \\ &+\frac{\mathrm{e}^{-\pi x/2}}{\pi^2 \beta J}\left[\mathrm{e}^{-\mathrm{i}\gamma\pi/2}\int \mathrm{e}^{-\xi} lA^{-}\,\mathrm{d}\xi + \mathrm{e}^{\mathrm{i}\gamma\pi/2}\int \mathrm{e}^{-\xi} l\bar{A}^{-}\,\mathrm{d}\xi\right].\end{aligned} \tag{34}$$

The crucial observation in [23] is that one needs not solve (33) to evaluate (34) provided that the kernel matrix function satisfies a symmetry, $\mathcal{K}_{i,j}(x-y) = \mathcal{K}_{j,i}(y-x)$. This property is valid in the present case. See (26).

We define $F_{\pm}$ by

$$\begin{aligned}F_{\pm} := \int_{-\infty}^{\infty} \sum_{p=1}^{k-1}\left[\left(\frac{\mathrm{d}}{\mathrm{d}\xi} ly_p^{\pm}\right) lY_p^{\pm} - \left(\frac{\mathrm{d}}{\mathrm{d}\xi} lY_p^{\pm}\right) ly_p^{\pm}\right]\mathrm{d}\xi + \int_{-\infty}^{\infty}\left[\left(\frac{\mathrm{d}}{\mathrm{d}\xi} la^{\pm}\right) lA^{\pm}\right.\\ \left. + \left(\frac{\mathrm{d}}{\mathrm{d}\xi} l\bar{a}^{\pm}\right) l\bar{A}^{\pm} - \left(\frac{\mathrm{d}}{\mathrm{d}\xi} lA^{\pm}\right) la^{\pm} - \left(\frac{\mathrm{d}}{\mathrm{d}\xi} l\bar{A}^{\pm}\right) l\bar{a}^{\pm}\right]\mathrm{d}\xi.\end{aligned} \tag{35}$$

Then the trick in [23] is as follows. First, take the derivative of both sides of (33) and multiply them by a row vector:

$$(lY_1^{\pm}(\xi), \ldots, lY_{k-1}^{\pm}(\xi), lA^{\pm}(\xi), l\bar{A}^{\pm}(\xi)). \tag{36}$$

We call the resultant equality (A). Second, multiply both sides of (33) by the derivative of the row vector (36), which is referred to as (B). Finally, subtract both sides of (A) and (B), and integrate over ξ. Then the lhs of the resultant equality is simply $F_{\pm}$. Remarkably, the most complicated terms in the rhs, such as

$$\int \mathrm{d}\xi\,\mathrm{d}\xi'\, lY_i^{+}(\xi)\frac{\mathrm{d}\bar{\mathcal{K}}_{i,j}\,(\xi-\xi')}{\mathrm{d}\xi} lY_j^{+}(\xi')$$

and

$$-\int \mathrm{d}\xi\, \mathrm{d}\xi'\, \frac{\mathrm{d}}{\mathrm{d}\xi} lY_j^+(\xi)\bar{\mathcal{K}}_{j,i}(\xi-\xi')lY_i^+(\xi')$$

cancel each other. To be precise, the first integral can be converted step by step,

$$\begin{aligned}
&= -\int \mathrm{d}\xi\, \mathrm{d}\xi'\, lY_i^+(\xi)\frac{\mathrm{d}\bar{\mathcal{K}}_{i,j}\,(\xi-\xi')}{\mathrm{d}\xi'} lY_j^+(\xi')\\
&= -\int \mathrm{d}\xi\, \mathrm{d}\xi'\, lY_i^+(\xi)\frac{\mathrm{d}\bar{\mathcal{K}}_{j,i}\,(\xi'-\xi)}{\mathrm{d}\xi'} lY_j^+(\xi')\\
&= \int \mathrm{d}\xi\, \mathrm{d}\xi'\, lY_i^+(\xi)\bar{\mathcal{K}}_{j,i}(\xi'-\xi)\frac{\mathrm{d}}{\mathrm{d}\xi'} lY_j^+(\xi')\\
&= \int \mathrm{d}\xi\, \mathrm{d}\xi'\, \frac{\mathrm{d}}{\mathrm{d}\xi} lY_j^+(\xi)\bar{\mathcal{K}}_{j,i}(\xi-\xi')lY_i^+(\xi')
\end{aligned}$$

where the symmetry of the kernel matrix, partial integration and the change of integration variables $\xi \leftrightarrow \xi'$ are used.

Similar cancellation happens for other terms and the following equality results:

$$F_\pm = 2\int [\mathrm{e}^{-\xi\pm \mathrm{i}\gamma\pi/2} lA^\pm + \mathrm{e}^{-\xi\mp \mathrm{i}\gamma\pi/2} l\bar{A}^\pm]\, \mathrm{d}\xi. \tag{37}$$

The first thermal correction (34) is thus given by

$$\frac{\mathrm{e}^{\pi x/2}F_+}{2\pi^2\beta J} + \frac{\mathrm{e}^{-\pi x/2}F_-}{2\pi^2\beta J}. \tag{38}$$

To evaluate $F_\pm$ explicitly, one rewrites the integration variable from ξ to $a, \bar{a}, y_p$. For example, the first summation term in $F_\pm$ is transformed to

$$\sum_{p=1}^{k-1}\int_{y_p^\pm(-\infty)}^{y_p^\pm(\infty)} \mathrm{d}y\, \left(\frac{\log(1+y)}{y} - \frac{\log y}{1+y}\right) = 2\sum_{p=1}^{k-1}\{L_+(y_p^\pm(\infty)) - L_+(y_p^\pm(-\infty))\}$$

and similarly for others. $L_+(x)$ is a dilogarithm function and is related to Rogers' dilogarithm function $L(x)$ by $L_+(x) = L(x/(1+x))$:

$$\begin{aligned}
L_+(x) &:= \frac{1}{2}\int_0^x \left(\frac{\log(1+y)}{y} - \frac{\log y}{1+y}\right) \mathrm{d}y\\
L(x) &:= -\frac{1}{2}\int_0^x \left(\frac{\log(1-y)}{y} + \frac{\log y}{1-y}\right) \mathrm{d}y
\end{aligned}. \tag{39}$$

The asymptotic values of scaling functions are easily extracted. For $x \to \infty$, $a^\pm$ coincides with original $\mathfrak{b}$. Thus, one derives the limiting value by its definition (19) in terms of $\lambda_p^{(k)}$. Similarly for $y_p^\pm(\infty)$. For $x \to -\infty$, one should rather consult (33). We send the argument $x \to -\infty$ in both sides and solve the resultant algebraic equations. The results are summarized as:

$$\begin{aligned}
&a^\pm(-\infty) = \bar{a}^\pm(-\infty) = 0 \qquad a^\pm(\infty) = \bar{a}^\pm(\infty) = k\\
&y_p^\pm(-\infty) = \frac{\sin\frac{\pi p}{k+2}\sin\frac{\pi(p+2)}{k+2}}{\sin^2\frac{\pi}{k+2}} \qquad 1 \leqslant p \leqslant k-1\\
&y_p^\pm(\infty) = p(p+2) \qquad 1 \leqslant p \leqslant k-1.
\end{aligned} \tag{40}$$

With these pieces of information, $F_\pm$ is now given by

$$F_+ = F_- = 2\sum_{p=1}^{k-1}\left[L\left(\frac{p(p+2)}{(p+1)^2}\right) - L\left(\frac{\sin\frac{\pi p}{k+2}\sin\frac{\pi(p+2)}{k+2}}{\sin^2\frac{\pi(p+1)}{k+2}}\right)\right] + 4L\left(\frac{k}{1+k}\right).$$

Finally we use three relations [39]:

$$L(1) = L(x) + L(1-x) = \frac{\pi^2}{6} \qquad x \in [0,1]$$

$$2L(1) = 2L\left(\frac{1}{n+1}\right) + \sum_{j=0}^{n-1} L\left(\frac{1}{(1+j)^2}\right) \qquad n \in Z_{\geqslant 0}$$

$$L(1)\frac{3n}{n+2} = \sum_{j=0}^{n-1} L\left(\frac{\sin^2\frac{\pi}{n+2}}{\sin^2\frac{\pi(j+1)}{n+2}}\right) \qquad n \in Z_{\geqslant 0}$$

which yield the neat result

$$F_{\pm} = \frac{\pi^2 k}{k+2}.$$

Thus we conclude the low-temperature asymptotics of the free energy:

$$f \sim e_0 - \frac{\pi}{6 v_s \beta^2} c(k) \qquad c(k) = 3k/(k+2) \tag{41}$$

where $v_s = J\pi/2$ coincides with the known spin velocity [40] and $c(k)$ is simply the central charge of the level-k $SU(2)$ WZWN model. This is the desired result from the WZWN description of massless quantum spin chains. We remark that the final part of the calculation is quite parallel to that in [11] utilizing the same dilogarithm function identities. There the spin-S XXZ model is discussed via the standard string approach at 'root of unity' where the number of strings is truncated finitely from the beginning.

7. Spinon characters

The character formulae obviously depend on the base of the space. Recently, the quasi-particle representation has attracted much attention in the context of the long-range interacting model [24, 41, 42], spectral decomposition of path space in lattice models [9], and in the statistical interacting picture of Bethe ansatz solvable models [43–47]. See also [48, 49] for different view points. For the spin-$\frac{1}{2}$ case, it has been recently shown that the novel thermodynamics formulation yields a natural spinon character and that such a character formula is generalized to $\widehat{\mathfrak{sl}}(n)_{k=1}$ [51]. Thus it is tempting to find analogues for $\widehat{\mathfrak{sl}}(n)_{k=2S}$. The results given in the previous sections provide the first step for the simplest $n = 2$ case as discussed below. Note that we consider 'chiral-half', such that the only positive contributions (say F_+) in the previous section are taken into account.

The character needs the description of all excited states. In the present context, this information might be encoded in the additional zeros of $\mathfrak{a}, \bar{\mathfrak{a}}, y$ and their capitals in their 'physical strips'. Indeed, some low excitations are identified in such a way [16, 18], and corresponding excited state TBAs are derived. Such an analysis is of considerable interest, however it requires extensive numerical efforts. We leave it as a future problem and make a short-cut detour here employing the strategy in [50].

The central charge is described by the dilogarithm function of which the integration contour is simple. On the other hand, one can define an analytically continued dilogarithm function $L_{\mathcal{C}}(z)$. This is established by adopting general contour $\mathcal{C}$ for the integration contour of the dilogarithm function. We then generalize a successful observation from specific examples; all excitation spectra, or effective central charge c_{eff}, in the conformal limit shall be described by $L_{\mathcal{C}}(z)$. Namely, the replacement of a simple contour in the integral representation of the dilogarithm function by a complex one leads to an excited state. Regarding c_{eff} as a function

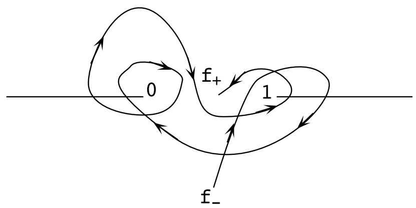

Figure 7. A contour $\mathcal{C}[f_-, f_+|\{2\}|\{-1, 1\}]$.

of $L_{\mathcal{C}}(z)$, the summation of $q^{-c_{\mathrm{eff}}/24}$ over a certain set of $\mathcal{C}$ is thus expected to reproduce affine characters. (Readers should not confuse this formal variable q, the standard notation in this field, with the Fourier variable used in previous sections.)

Let us be more precise. By $\mathcal{C}$ we denote a contour starting from f_- and terminating at f_+, such that it first crosses $[1, \infty)$ $\eta_1(\neq 0)$ times then crosses $(-\infty, 0]$ ξ_1 times then again η_2 times w.r.t. $[1, \infty)$ and so on. The intersections are counted as +1(−1) if the contour goes across the cut $[1, \infty)$ in the counterclockwise (clockwise) manner and $(-\infty, 0]$ in the clockwise (counterclockwise) manner. (Note that this definition is slightly different from [50, 51].) We denote this by $\mathcal{C}[f_-, f_+|\{\xi_1, \xi_2, \ldots\}|\{\eta_1, \eta_2, \ldots\}]$. The set of contours are parametrized by $\mathcal{S} = \{\mathcal{C}[f_-^{(p)}, f_+^{(p)}|\xi_1^{(p)}, \ldots, |\eta_1^{(p)}, \ldots,]\}$, where $f_\pm^{(p)} = y_p^+(\pm\infty)/Y_p^+(\pm\infty)$, $(1 \leqslant p \leqslant k-1)$, $f_+^{(k)} = \mathfrak{a}^+(\infty)/\mathfrak{A}^+(\infty)$, $f_+^{(k+1)} = \bar{\mathfrak{a}}^+(\infty)/\bar{\mathfrak{A}}^+(\infty)$ and $f_-^{(k)} = f_-^{(k+1)} = 0$.

In the absence of additional zeros of auxiliary functions in the 'physical strip', we have

$$0 = \log(f_+^{(p)}) - \sum_{p'} \mathfrak{g}_{p,p'} \log(1 - f_+^{(p')}) \tag{42}$$

where the 'statistical interaction' matrix $\mathfrak{g}$ is related to the zero mode of the Fourier transformation of the kernel matrix (26) by

$$\mathfrak{g} = I - \mathcal{K}[q = 0]. \tag{43}$$

This is the situation we have treated in previous sections, and (42) follows from (33). One replaces log in (42) by an analytically continued one, $\log_{\mathcal{C}}(z)$ in excited states:

$$\pi \mathrm{i} D^{(p)} = \log_{\mathcal{C}^{(p)}}(f_+^{(p)}) - \sum_{p'} \mathfrak{g}_{p,p'} \log_{\mathcal{C}^{(p')}}(1 - f_+^{(p')}) \tag{44}$$

where $\log_{\mathcal{C}^{(p)}}(f_+^{(p)}) = \log(f_+^{(p)}) - 2\pi \mathrm{i} \sum_\ell \xi_\ell^{(p)}$ and so on. Here $D^{(p)}$ is introduced for consistency of both sides, and is interpreted as 'chemical potential' [50]. On the other hand, $D^{(p)}$ should originate from the zeros of the auxiliary functions in the physical strips. One may be able to prove that such $D^{(p)}$ actually agree with ones in (44), in principle. Though such a microscopic derivation has yet to be performed, we assume the coincidence in the following.

The excitation spectrum is solely implemented in the effective central charge $c_{\mathrm{eff}}(\mathcal{S})$:

$$c_{\mathrm{eff}}(\mathcal{S}) = \frac{6}{\pi^2} \sum_p \left(L_{\mathcal{C}^{(p)}}(f_-^{(p)}, f_+^{(p)}) - \frac{\pi \mathrm{i}}{2} D^{(p)} \log_{\mathcal{C}^{(p)}}(1 - f_+^{(p)}) \right). \tag{45}$$

Here $D^{(p)}$ term is included by hand, so as to match its interpretation as chemical potential [50]. $L_{\mathcal{C}}$ is given by

$$L_{\mathcal{C}}(f_-, f_+) = -\frac{1}{2} \int_{\mathcal{C}} \left(\frac{\log_{\mathcal{C}}(1 - z)}{z} + \frac{\log_{\mathcal{C}}(z)}{1 - z} \right) \mathrm{d}z \tag{46}$$

for a path $\mathcal{C}$ from f_- to f_+.

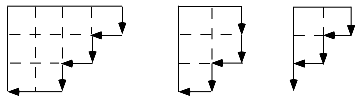

Figure 8. Young diagrams $YD^{(p)}$ of $n^{(p)} = 3$ corresponding to a set of winding numbers: $\{\xi\} = \{1,1,1\}, \{\eta\} = \{1,1,2\}$ (left), $\{\xi\} = \{1,1,1\}, \{\eta\} = \{0,1,1\}$ (middle) and $\{\xi\} = \{1,1,1\}, \{\eta\} = \{1,1,0\}$ (right). Arrows are included as a guide to the eye. The diagram on the far rhs is termed 'with tail' in the text.

After straightforward manipulations, one finds [50],

$$L_{\mathcal{C}^{(p)}}(f_-^{(p)}, f_+^{(p)}) = L(f_+^{(p)}) - L(f_-^{(p)}) - \pi\mathrm{i}\sum_\ell \xi_\ell^{(p)}\log(1-f_+^{(p)}) - \pi\mathrm{i}\sum_\ell \eta_\ell^{(p)}\log(f_+^{(p)})$$
$$+2\pi^2\left(\sum_\ell \xi_\ell^{(p)}\right)\left(\sum_\ell \eta_\ell^{(p)}\right) - 4\pi^2\sum_\ell \xi_\ell^{(a)}(\eta_1^{(a)}+\cdots+\eta_\ell^{(a)}). \tag{47}$$

Remember $L(z)$ is defined in (39). The substitution of (47) in (45), using (44) and the definitions of $\log_{\mathcal{C}^{(p)}}$ leads to a remarkable result: c_{eff} can only be written in terms of $c(k)$ (see (41)), $\{\xi_\ell^{(p)}\}$ and $\{\eta_\ell^{(p)}\}$,

$$c_{\mathrm{eff}}(\mathcal{S}) = c(k) - 24\mathcal{T}(\mathcal{S}) \qquad \mathcal{T}(\mathcal{S}) = \frac{1}{2}{}^t\boldsymbol{n}\mathfrak{g}\boldsymbol{n} + \sum_{a=1}^{k+1}\sum_{\ell\geqslant 1}\xi_\ell^{(a)}(\eta_1^{(a)}+\cdots+\eta_\ell^{(a)})$$
$${}^t\boldsymbol{n} = (n^{(1)},\ldots,n^{(k+1)}) \tag{48}$$

where $n^{(p)} = \sum_\ell \eta_\ell^{(p)}$. Note that the explicit forms of $D^{(p)}$ are not needed in the above transformation.

In the following, we shall argue that the summation of $q^{-c_{\mathrm{eff}}}$ over some subset $\mathcal{O}$ of all possible contours reproduce the character $\mathrm{ch}_j(z,q)$ of the level k WZWN model with spin-j ($j =$ some fixed integer or half-integer).

We present necessary conditions for such $\mathcal{O}$ below.

- η and ξ are non-negative.

Such a path can be parametrized by

$$\mathcal{C}[f_-^{(p)}, f_+^{(p)}|\xi_1^{(p)},\ldots,\xi_{n^{(p)}}^{(p)}|\underbrace{1,\ldots,1}_{n^{(p)}}]$$

and $\xi_\ell^{(p)} \geqslant 0$, $(p = 1,\ldots,n^{(p)})$.

- For $p = k, k+1$, we require $\frac{n^{(k)}+n^{(k-1)}}{2} - j \in \boldsymbol{Z}_{\geqslant 0}$ in addition.
- For $p \leqslant k-1$, $\xi_{n^{(p)}}^{(p)} \geqslant 1$.

Graphically, one can associate a Young diagram $YD^{(p)}$ to a set of winding numbers: $\{\xi_\ell^{(p)}\}, \{\eta_\ell^{(p)}\}$ (or a Young diagram with tail for some cases in $p = k, k+1$). First draw a line of length 1 downwards. Next draw a line of length $\xi_1^{(p)}$ to the left. Then draw a line of length 1 downwards again. We continue this procedure $n^{(p)}$ times. Finally draw a horizontal line from the starting point to the left and also draw a vertical line from the end point upwards. See figure 8. Obviously, the number of boxes in the diagram is equal to the second term in $\mathcal{T}(\mathcal{S})$.

We allow for contours which are isomorphic to a set of Young diagrams $YD^{(p)}$, $(p = 1,\ldots k-1)$ such that

- $n^{(k-2p+1)} =$ odd, $n^{(k-2p)} =$ even.
- By the definition, the depth of $YD^{(p)}$ is $n^{(p)}$. The width is restricted by the maximum value $w_{\max}^{(p)}$ which is determined by depths of 'adjacent' diagrams:
$$w_{\max}^{(p)} = \tfrac{1}{2}(n^{(p-1)} + n^{(p+1)} - 2n^{(p)} + \delta_{2j,k-p}) \qquad (p = 1, \ldots, k-2)$$
for the fixed j and $n^{(0)} = 0$. The case $p = k-1$ is exceptional: $w_{\max}^{(k-1)} = \frac{1}{2}(n^{(k-2)} + n^{(k)} + n^{(k+1)} - 2n^{(k-1)} + \delta_{j,1/2})$.

Under the above restrictions on $\mathcal{O}$, we find

$$\begin{aligned} q^{-\Delta(j)+j/2}\mathrm{ch}_j(z,q) &= \sum_{\mathcal{S}\in\mathcal{O}} q^{-c_{\mathrm{eff}}(\mathcal{S})/24} z^{(n^{(k)}-n^{(k+1)})/2} \\ &= \sum_{n^{(k)},n^{(k+1)}\geqslant 0} q^{-(n^{(k)}+n^{(k+1)})^2/4} \Psi_{A_k}^{n^{(k)}+n^{(k+1)}}(u_j;q)\mathcal{S}_{n^{(k)},n^{(k+1)}}(z;q). \end{aligned}$$

$\mathcal{S}_{M,N}(z;q)$ stands for contributions from (M,N) spinons:

$$\mathcal{S}_{M,N}(z;q) = \frac{1}{(q)_M(q)_N} z^{(M-N)/2}$$

resulting from summations over 'nodes' $\xi_\ell^{(p)} \geqslant 0$, $\ell = 1,\ldots,n^{(p)}$ and $p = k, k+1$. A_k is the Cartan matrix for sl_{k+1} and Ψ_{A_k} denotes

$$\Psi_{A_k}^{m_1}(u_j;q) = \sum_{m_2,m_3,\ldots,m_k} q^{1/4m\cdot A_k m} \prod_{i=2}^{k} \begin{bmatrix} \frac{1}{2}((2-A_k)\cdot m + u_j)_i \\ m_i \end{bmatrix}$$

and $(u_j)_i = \delta_{i,2j+1}$. The summations are taken over odd (even) positive integers for $m_{\mathrm{even(odd)}}$. Note we redefine $n^{(k-\ell)} = m_{\ell+1}$, $1 \leqslant \ell \leqslant k-1$. The appearance of the Gaussian q-binomial usually originates from combinatorics on the truncated Bratteli diagram and is the reminiscence of the RSOS model. Here the origin is also simple. It comes from the restriction on the width of Young diagrams. We denote the number of boxes in a Young diagram $YD^{(p)}$ by $b^{(p)}$. For fixed $\{n^{(a)}\}$, $\mathcal{T}(S)$ assumes the same value for diagrams having identical $b^{(p)}$. This multiplicity is given by $p(n^{(p)}, w_{\max}^{(p)}, b^{(p)}) =$ the number of partition of $b^{(p)}$ into at most $w_{\max}^{(p)}$ part, each $\leqslant n^{(p)}$. Thanks to the generating relation

$$\sum_{b^{(p)}} p(n^{(p)}, w_{\max}^{(p)}, b^{(p)}) q^{b^{(p)}} = \begin{bmatrix} n^{(p)} + w_{\max}^{(p)} \\ n^{(p)} \end{bmatrix} = \begin{bmatrix} (n^{(p-1)} + n^{(p+1)} + \delta_{p,k-2j})/2 \\ n^{(p)} \end{bmatrix}$$

we obtain the product of Gaussian q-binomial equivalent to the one in $\Psi_{A_k}^{m_1}(u;q)$.

Our result implies that the Hilbert space of the level-k $SU(2)$ WZWN model is isomorphic to a part of homotopy space of Rogers' dilogarithm function. We believe that this provides a novel interesting view point in the prototype of CFT and deserves further examinations.

8. Summary and discussion

In this paper, we formulate a novel description of the thermodynamics of solvable spin-S XXX models. The suitable choices of auxiliary functions yield a natural generalization of the strategy in [23]. The nonlinear integral equations close finitely, which differs clearly from the string formulation [2] and is obviously efficient in numerics. The resultant formulation has an interpretation in terms of physical excitations, spinons and RSOS kinks. This has been demonstrated by the calculation of the low-temperature specific heat as well as the spinon character formula. The latter, however, is derived under several assumptions on the possible homotopy class of $L_{\mathcal{C}}$. Certainly these constraints on winding numbers have 'microscopic' origins in patterns of zeros of $y-$ (or T) functions. This has actually been demonstrated for a few cases: the superintegrable 3-state chiral Potts model [52] and the simplest case of sl_2 RSOS models with open boundaries [53]. We hope to report on extensive numerical investigations on zeros in the present context in the near future.

Finally, we mention spinon pictures of different view points [54–56], where explicit 'spinon' bases have been constructed by vertex operators. Thus, the meaning of 'spinon' is more transparent than in our approach. Less obvious is their concrete relation to eigenstates of spin Hamiltonians. The method also involves an uncontrolled approximation, a truncation procedure, in evaluating the partition function as well as 'one body' distribution functions. This contrasts to the present approach which involves no approximation. In a sense they are complementary, and their relations are to be explored.

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