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The spectra of q-state vertex models and related antiferromagnetic quantum spin chains

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Abstract. Some exactly solvable q-state vertex models are investigated. We employ inversion relations to determine directly the spectra of the transfer matrices in the thermodynamic limit by avoiding the more cumbersome Bethe ansatz. The results are applied to related quantum spin chains of which two families are SU(q) and SO(q) invariant, respectively. Various quantities are calculated, e.g. energy–momentum excitations and the correlation length. For $q = 3$ the SU(q) invariant chain is the pure biquadratic spin-1 Hamiltonian which turns out to be non-critical. The ground-state energy, the gap, and the correlation length are given.

1. Introduction

We study the antiferromagnetic biquadratic spin-1 chain as well as some q-state vertex models ($q > 2$) and associated quantum spin chains. Some of the results we already reported in [1]. Renewed interest in quantum spin chains is due to Haldane's conjecture that integral-spin Heisenberg chains are non-critical, i.e. they have an excitation gap and a finite correlation length, in contrast to half-integer-spin Heisenberg chains [2, 3]. These ideas initiated a vivid study of the phase diagram of the bilinear–biquadratic spin-1 Hamiltonian [4–11] which is the most general SU(2) invariant three-state model with nearest-neighbour interaction

$$H_{\text{bilin-biquad}} = \sum_{j=1}^{N} [\cos\Theta\, \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + \sin\Theta\, (\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1})^2].$$

In the sector $\pi/2 \le \Theta \le 5\pi/4$ the model is ferromagnetic with a trivial ground state. The (spin-1) Sutherland model $\Theta = \pi/4$ is integrable and critical. It was solved first via a Bethe ansatz by Uimin [12] and then for arbitrary spin in [13]. Each local interaction of this Hamiltonian is basically the projector onto the triplet of two neighbouring spins. Furthermore the (spin-1) Takhtajan–Babujian model $\Theta = -\pi/4$ is exactly solvable [14, 15]. It is critical and conformally invariant [16–18]. For the point characterised by $\tan\Theta = 1/3$ there are also some exact results. The Hamiltonian here is the sum of all projectors onto the quintets of neighbouring spins and the ground state is a valence bond solid (VBS). The existence of a non-vanishing gap [9] is known as well as the two-spin correlation function which is decaying exponentially. This suggests that a massive phase does develop in the vicinity of the VBS point including

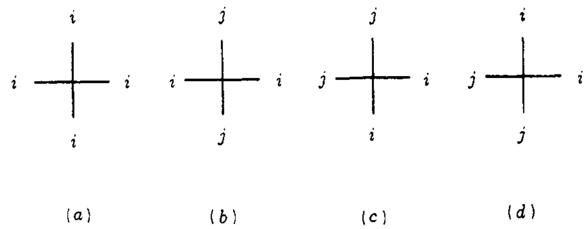


Figure 1. Representation of the four vertex types; the spin variables are $i \neq j = 1, \ldots, q$. To each class one Boltzmann weight is assigned, $a, \ldots, d$.

the Heisenberg chain $\Theta = 0$ in agreement with Haldane's conjecture. This is also supported by numerical results for finite chains [4–7, 10, 11].

Whether $\Theta = \pm\pi/4$ are the only critical points in the region $-3\pi/4 < \Theta < \pi/2$ remains unclear because of problems in obtaining definite results from finite lattice data. For the biquadratic chain $\Theta = -\pi/2$, where the Hamiltonian basically is the sum of the projectors onto the singlets of neighbouring spins, finite chain studies suggest a massless phase [7, 10] in contrast to a conjecture in [19]. However, it was shown in [1, 20] and independently in [21] (building on [22]) that there is a small but non-vanishing mass gap $\tilde{\Delta} = 0.173\,1788\ldots$. The large correlation length $\xi = 21.072\,8505\ldots$ [1] certainly explains the problems encountered in numerical works [7, 10, 11]. Similar results as for the biquadratic spin-1 Hamiltonian can be obtained for higher-spin models [1, 23, 24] which are also defined by projectors onto the singlet states of neighbouring spins.

The paper is organised as follows. In section 2 we define three families of exactly solvable q-state vertex models on a two-dimensional square lattice. For these classical models the partition function as well as the correlation length is derived. This is achieved within a transfer matrix approach by first setting up some functional relations in section 3 which provide a short-cut method [20, 25, 26] avoiding the more cumbersome Bethe ansatz [27–29]. The (inversion) relations are solved in the subsequent sections 4 and 5 yielding the largest eigenvalue and the next-largest eigenvalues of the transfer matrix. From this the partition function and the correlation length can be obtained. In section 6 one-dimensional quantum spin Hamiltonians are derived which are related to the two-dimensional classical vertex models. Among these models are the biquadratic spin-1 Hamiltonian and its generalisation to higher spins (family (1)) which is SU(q) invariant. This and a second family can be written as bilinear–biquadratic models in terms of SO(q) generators. The energy–momentum spectrum of the Hamiltonians is written down directly by exploiting expressions for the eigenvalues of the transfer matrices obtained in sections 4 and 5. Results are given for ground-state energy, excitations, gap and correlation length. A detailed proof of the inversion relation (10) can be found in the appendix.

2. Vertex models

We consider vertex models on a square lattice of M rows and N columns where M and N are assumed to be even and cyclic boundary conditions are imposed. To each bond a spin variable is attached which can take q (≥ 3) values $1, \ldots, q$. In this work only four types of vertex configurations are allowed which are depicted in figure 1. To all vertices of each type one Boltzmann weight a, b, c or d is assigned.

Exact results can be obtained for solutions of the star–triangle/Yang–Baxter equation [28]. We investigate three such solutions.

Solution (1):

$$\begin{aligned} a &= 1 \qquad c = \frac{\omega z + 1 - \omega}{z+1} \\ b &= 0 \qquad d = 1 - c = \frac{(1-\omega)z + \omega}{z+1} \end{aligned} \tag{1}$$

where

$$\omega := \frac{1}{2}\left(1 + \sqrt{\frac{q+2}{q-2}}\right)$$

is a constant and z is a (complex) variable. In what follows it will be sometimes useful to parametrise z as

$$z = \exp(\ln\alpha \cdot v) \tag{2}$$

where

$$\alpha := \left(\frac{\omega}{\omega - 1}\right)^2 = (q-2)^2\omega^4 \tag{3}$$

is a constant and v is the so-called spectral variable.

Solution (2):

$$\begin{aligned} a &= 1 - \frac{q-2}{2}\left(\frac{1}{4} - v^2\right) \qquad c = \frac{1}{2} + v \\ b &= \pm\frac{q-2}{2}\left(\frac{1}{4} - v^2\right) \qquad d = \frac{1}{2} - v \end{aligned} \tag{4}$$

where v is the spectral variable.

Solution (3):

$$\begin{aligned} a &= 1 \qquad c = \frac{(q-1)^{1/2} z - 1}{q-2} \\ b &= 0 \qquad d = \frac{(q-1)^{1/2} z^{-1} - 1}{q-2} \end{aligned} \tag{5}$$

where z is a variable which will be parametrised in the following as

$$z = \exp(\ln(q-1) \cdot v). \tag{6}$$

Models (1) and (3) for $q = 3$ were known to Stroganov [30] who derived the partition function in these cases by solving inversion relations. For the general cases (1)–(3) Perk and Schultz similarly calculated the partition function [31, 32]. In [32] some more exactly solvable models can be found within a classification of all solutions of the star–triangle equation for a more general class of vertex models than studied here. In [33, 34] the partition function was calculated again for cases (1) and (3) by mapping 'non-intersecting string models' onto the self-dual Potts model. Family (2) and its partition function were found first in [35], the Bethe ansatz equations were derived by an analytic ansatz in [36] and the algebraic Bethe ansatz was performed in [37].

Finally we wish to remark that the maximal (continuous) symmetry of the row-to-row transfer matrices of cases (1) and (2^-), i.e. case (2) with minus sign, is $SO(q)$. For cases (2^+) and (3) there is only the trivial symmetry $\{\mathrm{id}\}$.

3. Functional relations for the transfer matrix

In this section some properties of the row-to-row transfer matrix T are presented. The transfer matrix describes the contribution of a single row with fixed lower and upper spin configuration to the partition function. The matrix elements are polynomials in the Boltzmann weights (a, b, c, d). First a simple symmetry relation is derived from $T^T(a, b, c, d) = T(a, b, d, c)$. Since the weights c and d are interchanged for all families by the substitution $v \to -v$ we have $T^T(v) = T(-v)$ or

$$T^+(v) = T(-v^*). \tag{7}$$

A consequence of the star–triangle equation is the commutativity of all transfer matrices T for arbitrary spectral variables [28]

$$T(v)\, T(v') = T(v')\, T(v). \tag{8}$$

Equations (7) and (8) imply that $T(v)$ is normal and therefore diagonalisable. From (8) one then knows that the set of eigenvectors can be chosen independently of the spectral variable v. Hence each eigenvalue $\Lambda(v)$ has to share certain properties with the entries of the matrix $T(v)$ which are derived by inspection.

For families (2) and (3) each $\Lambda(v)$ is analytic.
For family (1) $\Lambda(v)$ is analytic up to poles of maximal order N at $v = (2n+1)\pi i/\ln\alpha$, n integer (corresponding to $z = -1$).
For families (1) and (3) each $\Lambda(v)$ has a period $2\pi i/\ln\alpha$ or $2\pi i/\ln(q-1)$, respectively.
For family (2) one has the asymptotic behaviour $\Lambda(v) \simeq (v^2)^N$, $v \to \pm i\infty$.

From (7) one immediately derives the symmetry relation

$$\Lambda^*(v) = \Lambda(-v^*). \tag{9}$$

At the special points $v = \mp 1/2$ the Boltzmann weights (a, b, c, d) are equal to (1,0,0,1) and (1,0,1,0). The corresponding transfer matrix reduces to a left- or right-shift operator, respectively. $T(-1/2)$ and $T(1/2)$ are inverse. A similar inversion relation is still valid in some neighbourhood of $v_0 = -1/2$

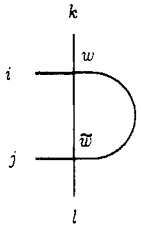
$$T(v) \cdot T(v+1) = \phi(v)^N I_N + \mathrm{O}(\mathrm{e}^{-N}) \tag{10}$$

where I_N is the identity matrix and $\mathrm{O}(\mathrm{e}^{-N})$ is a correction vanishing exponentially in the thermodynamic limit. ϕ is defined differently for the three cases:

$$\begin{aligned}
&(1) \qquad \phi(v) = \frac{\omega^2 \alpha z}{(z+1)(\alpha z+1)}(1-\alpha^{-1/2}z)(1-\alpha^{-3/2}z^{-1}) \\
&(2) \qquad \phi(v) = [1-(1/2+v)^2]\left[1-\left(\frac{q-2}{2}\right)^2(1/2+v)^2\right] \\
&(3) \qquad \phi(v) = \left(\frac{q-1}{q-2}\right)^2 [1-(q-1)^{-1/2}z][1-(q-1)^{-3/2}z^{-1}]
\end{aligned} \tag{11}$$

where z is parametrised by v according to (2) or (6). The proof of (10) is based on a vertex identity shown in figure 2 and is described in detail in the appendix. Equation (10) directly implies for the eigenvalues $\Lambda(v)$

$$\Lambda(v) \cdot \Lambda(v+1) = \phi(v)^N + \mathrm{O}(\mathrm{e}^{-N}). \tag{12}$$



$$= \quad \phi \cdot \delta(i,j) \cdot \delta(k,l)$$

Figure 2. Graphical representation of the vertex identity which is the keystone of the inversion relation. w is an arbitrary set of weights, $\tilde{w}$ and Φ are functions of w. On the left-hand side a summation must be performed over the spin variables of the inner bonds.

4. Largest eigenvalue of the transfer matrix and partition function

In this section the eigenvalue $\Lambda_0(v)$ which is largest in the physical region $-1/2 \leq \mathrm{Re}\,(v) \leq 1/2$ is determined. It is convenient to define

$$\psi(v) := \lim_{N\to\infty} \Lambda_0^{1/N}(v) \tag{13}$$

which has the meaning of the partition function per site. $\psi(v)$ can be calculated basically from the inversion relation as is standard by now [28, 30]. The required properties of $\psi(v)$ are:

(i) analyticity in the physical region $-1/2 \leq \mathrm{Re}\,(v) \leq 1/2$†, no zeros therein

(ii) periodicity/asymptotic behaviour (14)

(iii) inversion relation, $\psi(v)\psi(v+1) = \phi(v)$.

(In the case of the first family this scheme is slightly modified. $\psi(v)$ has poles of order 1 at $v = (2n+1)\pi\mathrm{i}/\ln\alpha$, n integer. From the inversion relation one can see with some effort that $\psi(v)$ is *anti*-periodic, $\psi(v + 2\pi\mathrm{i}/\ln\alpha) = -\psi(v)$‡. All difficulties could be removed by separating an overall weight factor $\sqrt{z}/(z+1)$ from the Boltzmann weights.)

There are two ways to proceed. For instance the first two properties of $\psi(v)$ enable one to write $\ln\psi(v)$ as a Fourier series/integral. The Fourier coefficients then can be read off from the inversion relation. An alternative way is to work out an ansatz for $\psi(v)$ taking into account all required properties. Then of course a uniqueness argument is needed. (Indeed the possibility of determining $\psi(v)$ via Fourier transform is such a proof. Nevertheless, it is easy to give an independent direct proof. Assume that there were two functions $\psi_1(v)$, $\psi_2(v)$ both exhibiting the properties listed above. Then $f(v) := \psi_1(v)/\psi_2(v)$ would be analytic and non-zero in a region containing the strip $-1/2 \leq \mathrm{Re}(v) \leq 1/2$. Using the inversion relation $f(v)$ can be continued analytically onto the whole complex plane. The continuation satisfies $f(v)f(v+1) = 1$. Therefore it is analytic and non-zero everywhere as well as 2-periodic. Since there is also an imaginary period or we have the asymptotic behaviour $f(v) \simeq$ constant, $v \to \pm\mathrm{i}\infty$, it follows that $f(v)$ is bounded on the whole complex plane. Due to Liouville's theorem $f(v)$ is constant and according to $f(v)f(v+1) = 1$ it is $+1$ or -1. The remaining

† By this, analyticity in some *open* region containing the strip $-1/2 \leq \mathrm{Re}(v) \leq 1/2$ is understood.

‡ This is allowed since $\psi(v)$ is a *root* of the periodic function $\Lambda_0(v)$.

ambiguity of the sign is irrelevant and can be lifted by requiring $\psi(v) > 0$ for physical values of v.)

Observing that $\psi(v)$ is real for real v the symmetry relation (9) applied to (13) yields

$$\psi(v) = \psi(-v). \tag{15}$$

This relation was not needed to prove the uniqueness of $\psi(v)$. It has to be satisfied automatically! (Note that $\phi(v) = \phi(-v-1)$ in (11). Then both functions $\psi_1(v) := \psi(v)$ and $\psi_2(v) := \psi(-v)$ possess all properties mentioned above. The uniqueness implies $\psi_1(v) = \psi_2(v)$.) Summarising we can say that the partition function per site $\psi(v)$ is determined by certain analyticity properties together with the inversion relation. The symmetry (15) in principal is not needed but may be used in actual calculations which are carried out below successively for the three models.

(1) Here a function $\psi(v)$ is calculated satisfying the inversion relation. The result will exhibit all necessary properties thus qualifying as the correct expression for the partition function. The symmetry property is taken into account by the ansatz

$$\psi(v) = \omega\,\alpha^{1/4}\frac{z^{1/2}}{z+1}F(z)\,F\left(\frac{1}{z}\right) \tag{16}$$

with an unknown function $F(z)$. Inserting (11) and (16) into (14) yields

$$\{F(z)\,F(\alpha z)\}\cdot\left\{F\left(\frac{1}{\alpha z}\right)F\left(\frac{1}{z}\right)\right\} = \{1-\alpha^{-1/2}z\}\{1-\alpha^{-1/2}(\alpha z)^{-1}\}. \tag{17}$$

This equation is satisfied if

$$F(z)\,F(\alpha z) = 1-\alpha^{-1/2}z. \tag{18}$$

Iterating the last equation one obtains

$$F(z) = \prod_{n=0}^{\infty}\frac{1-z/\alpha^{2n+3/2}}{1-z/\alpha^{2n+5/2}}. \tag{19}$$

This function is well defined and meromorphic on the whole complex plane. Indeed the function $\psi(v)$ defined by (16) and (19) is $(2\pi\mathrm{i}/\ln\alpha)$-antiperiodic, analytic up to simple poles (corresponding to $z=-1$), and non-zero in $-1/2 \le \mathrm{Re}\,(v) \le 1/2$.

(2) We employ the ansatz

$$\psi(v) = F(v)\,F(-v). \tag{20}$$

The inversion relation (14) is satisfied if

$$F(v)\,F(v+1) = \left(\frac{3}{2}+v\right)\left(\frac{q+2}{4}+\frac{q-2}{2}v\right). \tag{21}$$

The solution is

$$F(v) = \sqrt{2(q-2)}\,\frac{\Gamma(\frac{1}{2}v+\frac{5}{4})}{\Gamma(\frac{1}{2}v+\frac{3}{4})}\,\frac{\Gamma(\frac{1}{2}v+\frac{3}{4}+1/(q-2))}{\Gamma(\frac{1}{2}v+\frac{1}{4}+1/(q-2))}. \tag{22}$$

The function defined by (20) and (22) satisfies the required analyticity properties especially the asymptotic behaviour $\psi(v) \simeq v^2$, $v \to \pm i\infty$, which can be seen from $\Gamma(v+a)/\Gamma(v+b) \simeq v^{a-b}$.

(3) The ansatz

$$\psi(v) = \frac{q-1}{q-2} F(z) F\left(\frac{1}{z}\right) \tag{23}$$

satisfies the inversion relation (14) if

$$F(z) F((q-1)z) = 1 - (q-1)^{-1/2} z. \tag{24}$$

The correct solution is

$$F(z) = \prod_{n=0}^{\infty} \frac{1 - z/(q-1)^{2n+3/2}}{1 - z/(q-1)^{2n+5/2}}. \tag{25}$$

Equations (16), (19), (20), (22), (23) and (25) are the final result for the partition function per site $\psi(v)$. In section 6 the ground-state energy of the related quantum spin chain is calculated from $\psi(v)$.

5. Next-largest eigenvalues and correlation length

Here all eigenvalues $\Lambda(v)$ of the transfer matrix are determined for which

$$l(v) := \lim_{N\to\infty} \frac{\Lambda(v)}{\Lambda_0(v)} \tag{26}$$

is finite. The excitation function $l(v)$ must satisfy a simple inversion relation obtained by dividing equations (12) applied to $\Lambda(v)$ and $\Lambda_0(v)$: $l(v)\,l(v+1) = 1$. In the same way (9) gives rise to the symmetry relation $l^*(v) = l(-v^*)$. Following [20, 25, 26] the excitation function can be determined. The required properties of $l(v)$ are:

(i) analyticity in $-1/2 \le \mathrm{Re}(v) \le 1/2$, zeros are allowed
(ii) periodicity/asymptotic behaviour
(iii) inversion relation, $l(v)\,l(v+1) = 1$
(iv) symmetry relation, $l^*(v) = l(-v^*)$. (27)

The solution procedure is described in detail for case (1). Case (3) is very similar and case (2) can be treated after some slight modifications.

(1) The first property (analyticity) is an assumption made only for some region containing $-1/2 \le \mathrm{Re}(v) \le 1/2$. Using the inversion relation, however, the excitation function can be continued onto the whole complex plane. For simplicity this continuation is denoted also by $l(v)$. Since $l(v)$ has zeros in the physical region the continuation is a meromorphic function. Applying the inversion relation twice we obtain

$$l(v+2) = \frac{1}{l(v+1)} = l(v). \tag{28}$$

Therefore $l(v)$ has two independent periods 2 and $2\pi i/\ln\alpha$. A meromorphic function defined on the whole complex plane having two independent periods is an elliptic function. As is well known, it is determined up to a constant factor by its zeros and poles. We obtain

$$l(v) = C \prod_{j=1}^{\nu} \sqrt{k}\, \mathrm{snh}\, [K'(v - \Theta_j)] \tag{29}$$

where snh is the elliptic snh-function of modulus $k \in (0, 1)$ which is defined by requiring that the corresponding quarter-periods K, K' satisfy

$$K'/K = (\ln \alpha)/\pi. \tag{30}$$

(For definitions of elliptic functions and related quantities see the appendices of [25, 28].) Θ_j are the zeros of $l(v)$ in the physical region whose number is denoted by ν. (The identity (29) is proved by dividing the left-hand side by the product on the right-hand side. The ratio is an elliptic function without any zeros or poles. According to Liouville's theorem this function has to be constant.)

A simple argument shows that ν must be even. (Each snh factor on the right-hand side of (29) is $(2\pi\mathrm{i}/\ln\alpha)$-antiperiodic, but $l(v)$ is periodic.) Inserting (29) into the inversion relation one obtains $1 = l(v)\, l(v+1) = C^2 \cdot (\prod \cdots) = C^2 \cdot 1$ whereby C is determined: $C = \pm 1$. The final result for the excitation function $l(v)$ is

$$l(v) = \pm \prod_{j=1}^{\nu} \sqrt{k}\, \mathrm{snh}\, [K'(v - \Theta_j)]. \tag{31}$$

The location of zeros Θ_j is restricted by the symmetry relation $l^*(v) = l(-v^*)$. It implies that for each Θ_j there must be an Θ_i such that $\Theta_j = -\Theta_i^*$. In the simplest case $(i = j)$ this is satisfied if $\mathrm{Re}\,(\Theta_j) = 0$. Then there are no further restrictions on Θ_j and the excitation function is a superposition of free states. The Θ_j play the role of excitation parameters/rapidities whose number ν is even. In the following we assume that all values $\nu = 2, 4, \ldots$ are allowed (which can be proved, for example, for the six-vertex model). It is somewhat plausible that there are no bound states which would be characterised by 'complex conjugate' pairs $\Theta_j = -\Theta_i^*$ with $i \neq j$. (The Boltzmann weights do not possess a real period which is a necessary condition for bound states in the case of the six-vertex model. A rigorous proof, however, is still missing within this approach.)

(2) The reasoning here is basically the same as above. The only change is that one has to take into account the absence of an imaginary period. The asymptotic behaviour $l(v) \simeq$ constant, $v \to \pm\mathrm{i}\infty$, gives rise to the occurrence of tan factors in place of *snh* functions. The result is

$$l(v) = \pm \prod_{j=1}^{\nu} \tan[\tfrac{1}{2}\pi(v - \Theta_j)] \tag{32}$$

where $\nu = 2, 4, \ldots$ and the Θ_j are imaginary parameters.

(3) This case is very similar to case (1) where

$$l(v) = \pm \prod_{j=1}^{\nu} \sqrt{k}\, \mathrm{snh}\, [K'(v - \Theta_j)] \tag{33}$$

but here the modulus k is defined by

$$K'/K = [\ln(q-1)]/\pi. \tag{34}$$

By (30)–(34) all next-largest eigenvalues of the transfer matrix are given. In the next chapter the excitation functions are used for calculating the energy–momentum excitations of the related quantum spin chains.

Knowing the next-largest eigenvalues it is possible to derive the (vertical) correlation length [26, 38]. For cases (1) and (3) it is

$$\xi = -1/\ln k \tag{35}$$

where k is defined by (30) and (34), respectively. For case (2) the correlation length ξ is infinite. This ξ is the correlation length of vertically separated spins. It is independent of the spectral variable v. By substituting $v \to -v$ the lattice is rotated by an angle $\pi/2$. Therefore the vertical and horizontal correlation lengths are identical.

6. Quantum spin chains

Usually there is a one-dimensional quantum Hamiltonian H which is related to a two-dimensional classical model [28, 29]. For many exactly solvable models the Hamiltonian limit of the transfer matrix is performed at a special point v_0 of the spectral variable where $T(v_0)$ is a simple shift operator. (For our models v_0 is always equal to $-1/2$; see figure 3(a).) This guarantees that the derivative $T'(v_0)$ is a product of $T(v_0)$ and a sum of local interactions; see figure 3. Therefore the logarithmic derivative of $T(v)$ qualifies as a Hamiltonian

$$H = -(\ln T)'(v_0) = -\sum_{j=1}^{N} h_j \tag{36}$$

where h_j denotes a two-spin operator h acting on sites j and $j+1$. (The rotated vertex in figure 3(c) or (d) is the graphical representation of h.) The row (resp. column) index is given by an upper (resp. lower) combined index (β_1, β_2) (resp. (α_1, α_2)).

Case (1)

$$h^{(\beta_1,\beta_2)}_{(\alpha_1,\alpha_2)} = \frac{2\omega-1}{q+2}\ln\alpha\left[\delta(\alpha_1,\alpha_2)\delta(\beta_1,\beta_2) - \delta(\alpha_1,\beta_1)\delta(\alpha_2,\beta_2)\right].$$

Case (2^-). For the minus sign in (4) we have

$$h^{(\beta_1,\beta_2)}_{(\alpha_1,\alpha_2)} = -\tfrac{1}{2}(q-2)\delta(\alpha_1,\beta_2)\delta(\alpha_2,\beta_1) + \delta(\alpha_1,\alpha_2)\delta(\beta_1,\beta_2) - \delta(\alpha_1,\beta_1)\delta(\alpha_2,\beta_2).$$

Case (2^+). For the plus sign we have (37)

$$\begin{aligned} h^{(\beta_1,\beta_2)}_{(\alpha_1,\alpha_2)} = {} & -(q-2)\delta(\alpha_1,\alpha_2,\beta_1,\beta_2) + \tfrac{1}{2}(q-2)\delta(\alpha_1,\beta_2)\delta(\alpha_2,\beta_1) \\ & + \delta(\alpha_1,\alpha_2)\delta(\beta_1,\beta_2) - \delta(\alpha_1,\beta_1)\delta(\alpha_2,\beta_2). \end{aligned}$$

Case (3)

$$\begin{aligned} h^{(\beta_1,\beta_2)}_{(\alpha_1,\alpha_2)} = {} & \frac{\ln(q-1)}{q-2}[(q-2)\delta(\alpha_1,\alpha_2,\beta_1,\beta_2) + \delta(\alpha_1,\alpha_2)\delta(\beta_1,\beta_2) \\ & - (q-1)\delta(\alpha_1,\beta_1)\delta(\alpha_2,\beta_2)]. \end{aligned}$$

The δ symbol with four arguments is equal to 1 if all entries are identical, 0 otherwise.

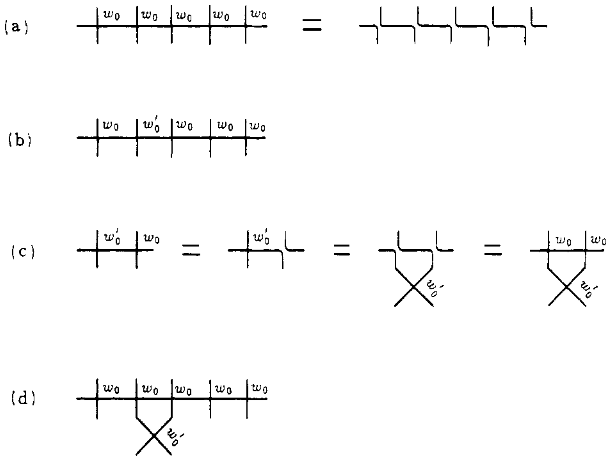


Figure 3. Graphical representation of identities which establish a relation of the transfer matrix $T(v)$ with some quantum spin chain H. w_0 denotes the set of weights (a, b, c, d) for the spectral variable $v_0 = -1/2$, w_0' denotes the derivatives of the weights with respect to v at v_0. According to (a) the matrix $T(v_0)$ is a shift operator. In (b) one of the summands of $T'(v_0)$ is depicted. Due to identity (c) the term (b) can be replaced by (d). (Note that in (c) and (d) a summation must be performed over the inner bonds.)

We want to add that in (36) periodic boundary conditions are used and that the momentum operator P (which is the generator of translations, e^{iP} = shift operator $= T(v_0)$) is given by

$$P = -i \ln T(v_0). \tag{38}$$

We briefly describe the symmetries of the Hamiltonians. The corresponding symmetry groups have to cover the symmetries of the transfer matrices but partly turn out to be bigger. The maximal symmetry of case (1) is $\mathrm{Sl}(q)$ (comprising $\mathrm{SU}(q)$ and $\mathrm{SO}(q)$) yet with different representations on even and odd sites. For case (2^-) the maximal symmetry is $\mathrm{SO}(q)$, for (2^+) it is the trivial group $\{\mathrm{id}\}$. Case (3) has a q-dimensional Abelian symmetry again with different representations on even and odd sites. Apparently the first two Hamiltonians can be written more nicely. Let $\boldsymbol{S}$ be the $q(q-1)/2$ vector of the generators of the group $\mathrm{SO}(q)$ which coincides for $q = 3$ with the usual $\mathrm{SU}(2)$ spin-1 operator. We then have

$$\begin{aligned}
&\text{Case (1)} \qquad H = -\frac{2\omega - 1}{q^2 - 4} \ln \alpha \sum_{j=1}^{N} [(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1})^2 - (q-1)] \\
&\text{Case } (2^-) \qquad H = \frac{1}{2(q-2)} \sum_{j=1}^{N} [(q-2)^2 (\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}) + (q-4)(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1})^2 + q].
\end{aligned} \tag{39}$$

The first Hamiltonian can be formulated furthermore in a simple way in terms of $\mathrm{SU}(2)$ spin-s operators $\boldsymbol{s}_j$ (with $2s + 1 = q$)

$$\text{Case (1)} \qquad H = -\frac{2\omega - 1}{q + 2} \ln \alpha \sum_{j=1}^{N} P[(\boldsymbol{s}_j + \boldsymbol{s}_{j+1})^2] \tag{40}$$

where the polynomial $P[\cdots]$ basically describes a projection onto the singlet state of the neighbouring spins

$$P[x] = -1 + q \prod_{j=1}^{2s} \left(1 - \frac{x}{j(j+1)}\right). \tag{41}$$

By (36) and (38) the Hamiltonian H and the momentum operator P are related to $T(v)$. Therefore all energy–momentum eigenvalues can be derived from the spectrum of $T(v)$. The ground-state energy $\varepsilon_0 := \lim_{N\to\infty} E_0/N$ is determined by the partition function (per site)

$$\varepsilon_0 = -(\ln \psi)'(v_0). \tag{42}$$

More interesting are the (low-lying) energy–momentum excitations which are calculated from the excitation function $l(v)$

$$\begin{aligned} E - E_0 &= -(\ln l)'(v_0) \\ P - P_0 &= -\mathrm{i} \ln l(v_0). \end{aligned} \tag{43}$$

Since $l(v)$ is a product of independent factors the excitations turn out to be sums of independent elementary momenta and energies, p_i and $\varepsilon(p_i)$

$$\begin{aligned} E - E_0 &= \sum_{i=1}^{\nu} \varepsilon(p_i) \\ P - P_0 &= \sum_{i=1}^{\nu} p_i \end{aligned} \tag{44}$$

where the dispersion $\varepsilon(p)$ is given by

$$\begin{aligned} &(1),(3) \qquad \varepsilon(p) = K' \sqrt{(1-k)^2 + 4k \sin^2 p} \\ &(2) \qquad \varepsilon(p) = \pi |\sin p|. \end{aligned} \tag{45}$$

(k, K' are defined differently for cases (1) and (3)!)

Obviously the Hamiltonian of case (1) has a gap $\varepsilon(0)$ multiplied by the minimal value of ν which is 2

$$(1) \qquad \Delta = 2\varepsilon(0) = 2K'(1-k) = \ln(\alpha) \prod_{n=1}^{\infty} \left(\frac{1-(1/\alpha)^{n/2}}{1+(1/\alpha)^{n/2}}\right)^2 \tag{46}$$

where α is defined in (3). The Hamiltonians of case (2) are gapless. In case (3) the gap is

$$(3) \qquad \Delta = \ln(q-1) \prod_{n=1}^{\infty} \left(\frac{1-(q-1)^{-n/2}}{1+(q-1)^{-n/2}}\right)^2. \tag{47}$$

These results are consistent with the findings for the correlation length ξ which is the same as for the corresponding vertex model, see (35). Therefore cases (1) and (3) are non-critical and case (2) is critical for all $q > 2$.

We discuss now the Hamiltonians (1) and (2^-) for the lowest value $q = 3$. For this value both Hamiltonians (1) and (2^-) turn out to be special cases of the bilinear-biquadratic spin-1 Hamiltonian, see (39). Model (1) essentially is the biquadratic Hamiltonian, $\tilde{H} = -\sum (\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1})^2$. From (16) and (42) the ground-state energy can be calculated numerically

$$\tilde{\varepsilon}_0 = -2.796\,863\ldots \quad (48)$$

The biquadratic Hamiltonian is non-critical since it has a non-zero energy gap $\tilde{\Delta}$ and a finite correlation length ξ which proves the conjecture of [19]. $\tilde{\Delta}$ can be calculated from (46) by taking into account the scale factor for $\tilde{H}$

$$\tilde{\Delta} = \sqrt{5}\prod_{n=1}^{\infty}\left(\frac{1-(1/\alpha)^{n/2}}{1+(1/\alpha)^{n/2}}\right)^2 = 0.173\,1788\ldots \quad (49)$$

where $\alpha = [\frac{1}{2}(1+\sqrt{5})]^4$ was inserted. From (35) we obtain the correlation length

$$\xi = -1/\ln k = 21.072\,8505\ldots \quad (50)$$

where k was calculated from requirement (30) and from standard formulae for elliptic quantities; see the appendices of [25, 28]. These results, notably (48) and (49), have been found independently also by Barber and Batchelor by using a quite different method [21] thereby clarifying and extending the observations made by Parkinson [22]. The rather large value of the correlation length (50) may explain the difficulties in drawing definite conclusions from the numerical treatment of finite chains. The largest chain considered in [11] had length 26! The degeneracy of the ground state which could not be determined within our approach is expected on physical grounds to be twofold due to dimerisation.

The second Hamiltonian (2^-) coincides for $q = 3$ with the (spin-1) Takhtajan–Babujian model $\Theta = -\pi/4$ [14, 15]. The ground-state energy and the dispersion (45) confirm known results [14].

Very recently the work in [21] was extended to higher-spin chains [23, 24] which are identical with family (1) for arbitrary q. In [23, 24] these q-state models could be mapped to the quantum Hamiltonian limit of the q^2-state Potts model for finite chains with free ends and finally to the Bethe-ansatz solvable spin-1/2 XXZ model. The conclusions of [23, 24] are in accordance with our findings [1].

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$$M(k,l)^{(i,j)}_{(m,n)} :=$$

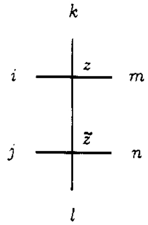

Figure 4. Definition of the matrices $M(k,l)$. (i, j) is a combined row index, (m, n) the column index, $i, j, k, l, m, n = 1,\ldots,q$. On the right-hand side a summation over the inner bond must be performed.

Appendix

In this appendix the inversion relation (10) is proved. Some $q^2 \times q^2$ matrices $M(k,l)$ $(k,\ l = 1,\ldots,q)$ are defined graphically in figure 4. The argument $(k,\ l)$ specifies one of these matrices (whose number is q^2); it is no row or column index.

First one has to prove the existence of a $q^2 \times q^2$ matrix V such that

$$V^{-1}M(k,l)\,V = \begin{pmatrix} \gamma(k,l) & * & \cdot & \cdot & \cdot & * \\ 0 & & & & & \\ \cdot & & & & & \\ \cdot & & & O(v-v_0) & & \\ \cdot & & & & & \\ 0 & & & & & \end{pmatrix} \tag{A1}$$

where

$$\gamma(k,l) := \begin{cases} \phi(v) & k = l \\ 0 & \text{otherwise} \end{cases} \tag{A2}$$

and $O(v - v_0)$ is a $(q^2 - 1) \times (q^2 - 1)$ matrix whose elements are analytic functions of v and possess a zero at $v_0 = -1/2$. For this proof define a q^2 vector X by

$$X_{(m,n)} := \delta(m,n). \tag{A3}$$

$X_2,\ldots,X_{q^2}$ may be some completion such that $X, X_2,\ldots,X_{q^2}$ are linearly independent. Define

$$V := (X, X_2,\ldots,X_{q^2}). \tag{A4}$$

For $v = v_0$ we have

$$M_0(k,l)^{(i,j)}_{(m,n)} = \delta(i,j)\delta(k,m)\delta(l,n). \tag{A5}$$

Hence all columns of $M_0(k,l)$ are multiples of X so that

$$M_0(k,l)\cdot V = V\cdot \begin{pmatrix} * & \cdot & \cdot & \cdot & * \\ 0 & & & & \\ \cdot & & & & \\ \cdot & & 0 & & \\ \cdot & & & & \\ 0 & & & & \end{pmatrix} \tag{A6}$$

where each $*$ denotes a suitable (complex) number. Due to the analyticity of the elements of $M(k,l)$

$$M(k,l)\cdot V = V\cdot\begin{pmatrix} * & \cdot & \cdot & \cdot & * \\ \cdot & & & & \\ \cdot & & O(v-v_0) & & \\ \cdot & & & & \\ * & & & & \end{pmatrix}. \tag{A7}$$

According to the vertex identity represented in figure 2, X is an eigenvector of $M(k,l)$ with eigenvalue $\gamma(k,l)$. Therefore the first column of $M(k,l)\cdot V$ must be identical to $\gamma(k,l)\cdot X$. Using (A7) this implies

$$M(k,l)\cdot V = V\cdot\begin{pmatrix} \gamma(k,l) & * & \cdot & \cdot & \cdot & * \\ 0 & & & & & \\ \cdot & & & & & \\ \cdot & & & O(v-v_0) & & \\ \cdot & & & & & \\ 0 & & & & & \end{pmatrix} \tag{A8}$$

which proves (A1).

In order to prove finally (10) one has to observe that $T(v)\,T(v+1)$ basically is a product of N matrices M_p of the kind $M(k,l)$:

$$\begin{aligned} T(v)\,T(v+1) &= \mathrm{Tr}\left(\prod_{p=1}^{N} M_p\right) = \mathrm{Tr}\left(\prod_{p=1}^{N} V^{-1}M_p V\right) \\ &= \mathrm{Tr}\begin{pmatrix} \prod_{p=1}^{N}\gamma_p & * & \cdot & \cdot & \cdot & * \\ 0 & & & & & \\ \cdot & & & & & \\ \cdot & & & O(v-v_0) & & \\ \cdot & & & & & \\ 0 & & & & & \end{pmatrix} \\ &= \prod_{p=0}^{N}\gamma_p + O((v-v_0)^N) \\ &= \begin{cases} \phi(v)^N + O((v-v_0)^N) & \text{if all upper and lower indices are identical} \\ O((v-v_0)^N) & \text{otherwise.} \end{cases} \end{aligned} \tag{A9}$$

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