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Optimum ground states for spin- $\frac{3}{2}$ ladders with two legs*

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Received 1 September 1998

Abstract. We construct the exact ground state for an antiferromagnetic spin- $\frac{3}{2}$ model on the two-leg ladder as an *optimum ground state*. The ground state contains a discrete parameter $\sigma = \pm 1$ and a continuous parameter a which controls z -axis anisotropy. For most values of a the global ground state is unique. It has vanishing sublattice magnetization and exponentially decaying correlation functions. By using the transfer matrix technique, we calculate exactly the fluctuations of the magnetization, the nearest-neighbour correlation, and the longitudinal correlation length as functions of the parameters.

1. Introduction

The investigation of quantum spin ladders is a very active field of condensed matter physics. Reports concerning experimental realizations of such systems are contributed frequently, see for instance [1–5]. A review can be found in [6]. From a theoretical point of view, spin ladders have been investigated by using exact diagonalization [7], density matrix renormalization group (DMRG) methods [8, 9], bosonization [10], and various other techniques, see e.g. [11–13] and references therein.

Recently, Kolezhuk and Mikeska [14] presented a set of *matrix product ground states* for special isotropic spin- $\frac{1}{2}$ ladder models. To each rung of the ladder, a matrix is assigned, which has local spin states for the corresponding rung as its elements. The global state is given by the product of these matrices, in which the matrix elements are multiplied via the tensorial product in spin space. If the model parameters obey the conditions given in [14], the resulting global state is a so-called *optimum ground state*, i.e. it is not only a ground state of the global Hamiltonian, but also of every local interaction operator.

In this paper we construct a one-parametric set of optimum ground states for antiferromagnetic spin- $\frac{3}{2}$ ladders with two legs. The local interaction is identical to the one on the hexagonal lattice in our previous paper [15]. In contrast to [14], the global ground state is given in terms of a *vertex state model*, which is a generalization of the MPG approach. This allows us to specify the local spin states for every lattice site instead of for complete rungs as required by the MPG approach. Properties of the ground state are calculated by using the *transfer matrix technique*, which is explained in the appendix.

* Dedicated to Professor H Horner on the occasion of his 60th birthday.

2. The model

Consider a ladder of length L with two legs and periodic boundary conditions. Each lattice site is occupied by a spin- $\frac{3}{2}$. The global Hamiltonian

$$H = \sum_{i=1}^L [h_{i,i+1} + h_{i',i'+1} + h_{i,i'}] \quad (1)$$

contains only nearest-neighbour interactions. If the ladder is visualized horizontally, the index i (i') denotes the upper (lower) spin on rung number i . All local interactions are equal: they only act on different spin pairs, i.e. the system is completely homogeneous.

The local interaction operator is the same as in the spin- $\frac{3}{2}$ model on the hexagonal lattice presented in our previous paper [15]. It is given in terms of projectors onto its eigenstates:

$$h_{ij} = \lambda_3(|v_3\rangle\langle v_3| + |v_{-3}\rangle\langle v_{-3}|) + \lambda_2^{-\sigma}(|v_2^{-\sigma}\rangle\langle v_2^{-\sigma}| + |v_{-2}^{-\sigma}\rangle\langle v_{-2}^{-\sigma}|) \\ + \lambda_{12}^+(|v_{12}^+\rangle\langle v_{12}^+| + |v_{-12}^+\rangle\langle v_{-12}^+|) + \lambda_{02}^{-\sigma}|v_{02}^{-\sigma}\rangle\langle v_{02}^{-\sigma}| \quad (2)$$

where

$$\begin{aligned} |v_3\rangle &= |33\rangle \\ |v_{-3}\rangle &= |\bar{3}\bar{3}\rangle \\ |v_2^{-\sigma}\rangle &= |31\rangle - \sigma|13\rangle \\ |v_{-2}^{-\sigma}\rangle &= |\bar{3}\bar{1}\rangle - \sigma|\bar{1}\bar{3}\rangle \\ |v_{12}^+\rangle &= a|11\rangle - (|3\bar{1}\rangle + |\bar{1}3\rangle) \\ |v_{-12}^+\rangle &= a|\bar{1}\bar{1}\rangle - (|\bar{3}\bar{1}\rangle + |\bar{1}\bar{3}\rangle) \\ |v_{02}^{-\sigma}\rangle &= \sigma a^2(|1\bar{1}\rangle - \sigma|\bar{1}1\rangle) - (|3\bar{3}\rangle - \sigma|\bar{3}\bar{3}\rangle). \end{aligned} \quad (3)$$

$\lambda_3, \lambda_2^{-\sigma}, \lambda_{12}^+, \lambda_{02}^{-\sigma}$ are positive real numbers, a is real, and $\sigma = \pm 1$. The canonical spin- $\frac{3}{2}$ basis states are denoted as

$$\begin{aligned} S^z|3\rangle &= \frac{3}{2}|3\rangle & S^z|\bar{3}\rangle &= -\frac{3}{2}|\bar{3}\rangle \\ S^z|1\rangle &= \frac{1}{2}|1\rangle & S^z|\bar{1}\rangle &= -\frac{1}{2}|\bar{1}\rangle. \end{aligned} \quad (4)$$

Note that (2) has the following properties.

- (1) It has rotational symmetry in the xy -plane of spin space, i.e. it commutes with the local magnetization operator $S_i^z + S_j^z$.
- (2) It is parity-invariant, i.e. it commutes with the operator P_{ij} , which interchanges the spins at lattice sites i and j .
- (3) It has spin-flip symmetry, i.e. it is invariant under the transformation $S^z \rightarrow -S^z$.
- (4) Its lowest eigenvalue is zero, i.e. h_{ij} is positive semidefinite.

The Hamiltonian contains five continuous parameters, namely four λ -parameters plus a . This includes a trivial scale. The two-spin states (3) are the excited local eigenstates of h_{ij} , the remaining nine eigenstates are local ground states, i.e. the corresponding eigenvalue is zero.

Since the global Hamiltonian (1) is a sum of positive semidefinite operators, zero is also a lower bound of the global ground state energy E_0 . In the next section a global eigenstate corresponding to eigenvalue zero is constructed, which must therefore be the global ground state.

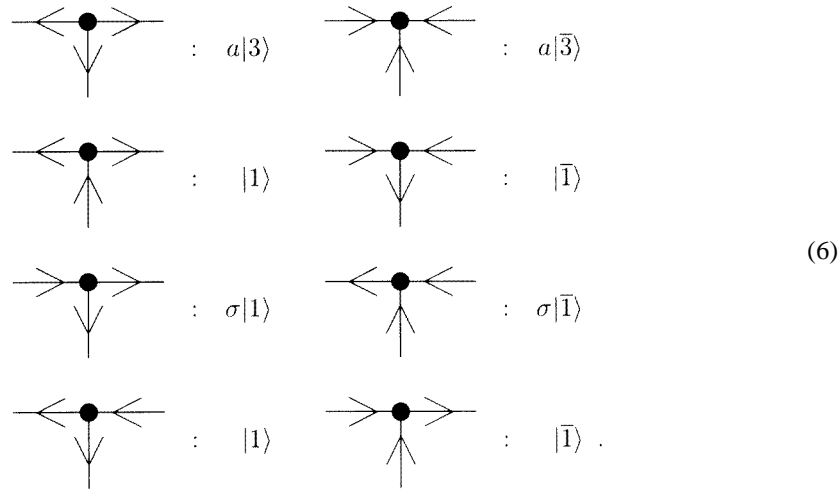
For $a = -\sqrt{3}$ and $\sigma = -1$, the λ -parameters can be chosen so that (3) are eigenstates of $(\mathbf{S}_i + \mathbf{S}_j)^2$. In this *isotropic case*, the local interaction (2) has complete $SO(3)$ symmetry in spin space and can be written as

$$h_{ij} = \mathbf{S}_i \cdot \mathbf{S}_j + \frac{116}{243}(\mathbf{S}_i \cdot \mathbf{S}_j)^2 + \frac{16}{243}(\mathbf{S}_i \cdot \mathbf{S}_j)^3 + \frac{55}{108} \quad (5)$$

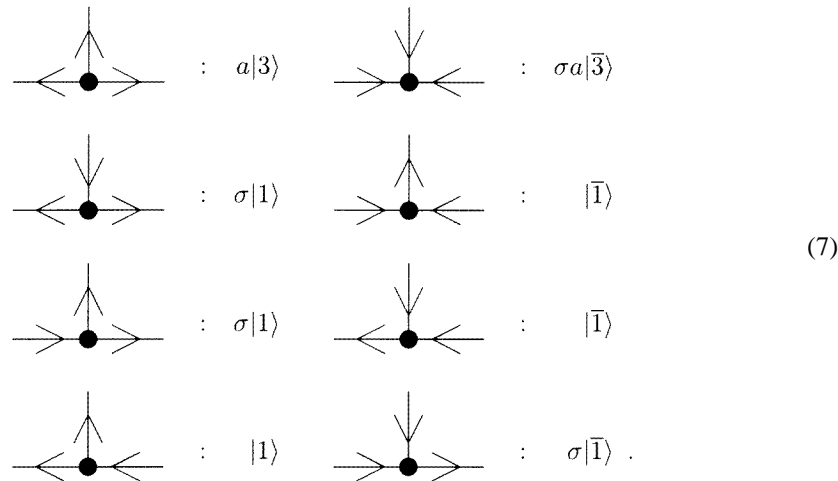
which simply projects onto all states with $(\mathbf{S}_i + \mathbf{S}_j)^2 = 3(3 + 1)$.

3. The global ground state

To each lattice site we assign a set of *vertices* with binary bond variables which are denoted as arrows. The values of these vertices are single-spin states at the corresponding lattice site. On the upper row



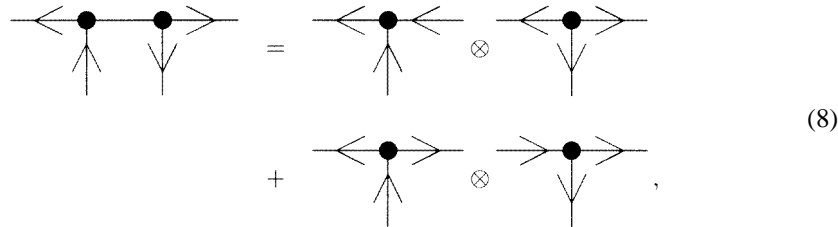
On the lower row



The parameters a and σ are the same as in (3).

In order to construct the global ground state from these local spin states, it is necessary to define the concatenation of the vertices (6) and (7), respectively. This is similar to

classical vertex models of statistical physics, but the generic product of numbers is replaced by the tensorial product in spin space:



$$(8)$$

i.e. the interior bond between the two vertices is summed out. Concatenations between adjacent vertices on the lower row and between upper and lower vertex on the same rung are completely analogous. The resulting cluster represents a state in the Hilbert space of two neighbouring spins.

A global state $|\Psi_0\rangle$ can be constructed by successively attaching vertices to the cluster until the ladder has the desired length. This process is associative, i.e. the order in which the vertices are concatenated does not matter. As periodic boundary conditions are imposed, the ‘free’ bonds at the first and last rung of the ladder have to be summed out. Because of the similarity to classical vertex models, such a global state is called a *vertex state model* [15, 17]. These are direct generalizations of the well known *matrix product ground states* for spin chains [16, 17]. If $|\varphi_i^{\mu_1\mu_2\mu_3}\rangle$ denotes the vertex at site i with arrow variables μ_1 , μ_2 , and μ_3 (cf definitions (6) and (7)), a formal expression for the ground state is given by

$$|\Psi_0\rangle = \sum_{\{\mu\}} \prod_i |\varphi_i^{\mu_1\mu_2\mu_3}\rangle. \quad (9)$$

The sum is over all arrow configurations on the bonds.

In order to show that the resulting global state $|\Psi_0\rangle$ is the ground state of the Hamiltonian (1), we collect all two-spin states which are generated by all possible concatenations of two vertices[†]:

$$\begin{aligned} |31\rangle + \sigma|13\rangle & \quad \overline{|3\bar{1}}\rangle + \sigma\overline{|1\bar{3}}\rangle \\ |11\rangle + a|3\bar{1}\rangle & \quad \overline{|1\bar{1}}\rangle + a\overline{|3\bar{1}}\rangle \\ |11\rangle + a|\bar{1}3\rangle & \quad \overline{|1\bar{1}}\rangle + a|\bar{1}\bar{3}\rangle \\ |\bar{1}\bar{1}\rangle + \sigma a^2|\bar{3}\bar{3}\rangle & \quad \overline{|\bar{1}\bar{1}}\rangle + \sigma a^2\overline{|\bar{3}\bar{3}}\rangle \\ |\bar{1}\bar{1}\rangle + \sigma|\bar{1}\bar{1}\rangle & \end{aligned} \quad (10)$$

It is easy to check that each of these nine two-spin states is perpendicular to all local excited states (3), i.e. they are annihilated by the local interaction operator (2). In other words, (10) are the local ground states of h_{ij} .

From the construction of the vertex state model it is clear that any projection of $|\Psi_0\rangle$ onto the Hilbert space of two neighbouring spins is a linear combination of the two-spin states (10). Therefore $|\Psi_0\rangle$ is annihilated by all local interaction operators,

$$h_{ij}|\Psi_0\rangle = 0 \quad (11)$$

for all nearest neighbours i and j . Hence

$$H|\Psi_0\rangle = 0. \quad (12)$$

As explained above, zero is a lower bound for the ground state energy E_0 , therefore $|\Psi_0\rangle$ must be the ground state of H . This type of global ground state, which simultaneously

[†] Common prefactors have been omitted.

minimizes all local interaction operators, is called an *optimum ground state* [15–17], since E_0 takes the lowest possible value.

4. Properties of the ground state

The first interesting expectation value is the magnetization of a single spin. As can be seen from the vertices (6) and (7), a spin flip $S^z \rightarrow -S^z$ is equivalent to a flip of all arrows on the bonds, which leaves the global state invariant. Therefore the single-spin magnetization $\langle S_i^z \rangle_{\Psi_0}$ must vanish. In this sense the global ground state is antiferromagnetic.

For $a \rightarrow \infty$, the structure of the global ground state becomes very simple. In this limit, the ground state is completely dominated by the vertices

$$\begin{array}{ccc}
 \begin{array}{c} \leftarrow \bullet \rightarrow \\ \downarrow \\ \leftarrow \bullet \rightarrow \end{array} : a|3\rangle & \begin{array}{c} \rightarrow \bullet \leftarrow \\ \uparrow \\ \rightarrow \bullet \leftarrow \end{array} : a|\bar{3}\rangle & \\
 \begin{array}{c} \uparrow \\ \leftarrow \bullet \rightarrow \\ \downarrow \\ \leftarrow \bullet \rightarrow \end{array} : a|3\rangle & \begin{array}{c} \downarrow \\ \rightarrow \bullet \leftarrow \\ \uparrow \\ \rightarrow \bullet \leftarrow \end{array} : \sigma a|\bar{3}\rangle & .
 \end{array} \tag{13}$$

Clearly, there are only two different possibilities to concatenate these four vertices to form a global state. These two possibilities correspond to the two different Néel states on the ladder. Thus in the limit $a \rightarrow \infty$, the global ground state is simply given by†

$$|\Psi_0\rangle = |\text{Néel}_1\rangle + \sigma^L |\text{Néel}_2\rangle. \tag{14}$$

The *transfer matrix technique* can be used to calculate expectation values for arbitrary values of the parameters a and σ . The appendix explains how to apply this method to the two-leg ladder. For the present model, the eigensystem of the transfer matrix can be obtained exactly, but has a very complicated form. For this reason, explicit formulae for the expectation values have been omitted. Instead, the results for the thermodynamic limit are plotted as a function of the parameter a . The dependence on σ drops out in all expectation values, which are calculated in this work.

Consider the combined magnetization operator of an elementary cell at rung number i ,

$$\tilde{S}_i^z = S_i^z + S_{i'}^z \tag{15}$$

where the index i/i' again denotes the upper/lower spin on the rung, respectively. Of course, $\langle \tilde{S}_i^z \rangle_\infty$ vanishes. Its fluctuations can be calculated by using equation (A.6). The result is shown in figure 1. The maximum at $a \approx 1.4$ can be understood as follows: it is clear from the vertices (6) and (7), that for $a = 0$ the system contains only the single-spin states $|1\rangle$ and $|\bar{1}\rangle$. With increasing values of a , $|3\rangle$ and $|\bar{3}\rangle$ states are mixed in, so the fluctuations become larger. Finally, for $a \rightarrow \infty$, the global ground state is simply a superposition of both possible Néel states, so the system is frozen. Therefore, the fluctuations must vanish in this limit.

Correlations between two different rungs can be obtained from equation (A.7). The nearest-neighbour correlation, $\langle \tilde{S}_i^z \tilde{S}_{i+1}^z \rangle_\infty$, is plotted as a function of a in figure 2. The shape is very similar to the one in figure 1. Note that the correlation is antiferromagnetic for all values of a . The vanishing in the limit $a \rightarrow \infty$ becomes clear from

$$\langle \tilde{S}_i^z \tilde{S}_{i+1}^z \rangle_\infty = \langle S_i^z S_{i+1}^z \rangle_\infty + \langle S_{i'}^z S_{i+1'}^z \rangle_\infty + \langle S_i^z S_{i+1'}^z \rangle_\infty + \langle S_{i'}^z S_{i+1}^z \rangle_\infty. \tag{16}$$

† The global prefactor a^{2L} has been dropped.

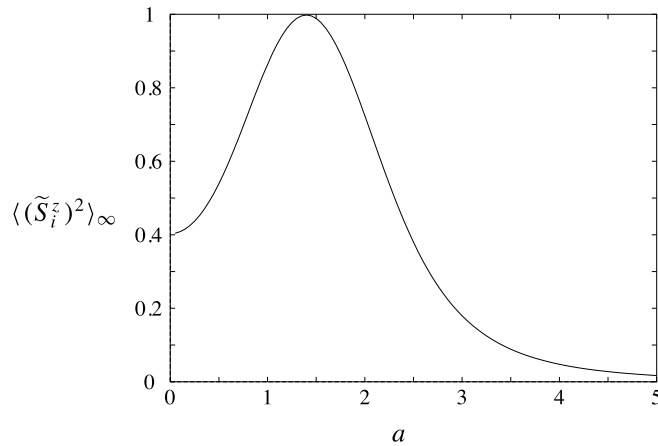


Figure 1. Fluctuations of the pair magnetization as a function of the parameter a .

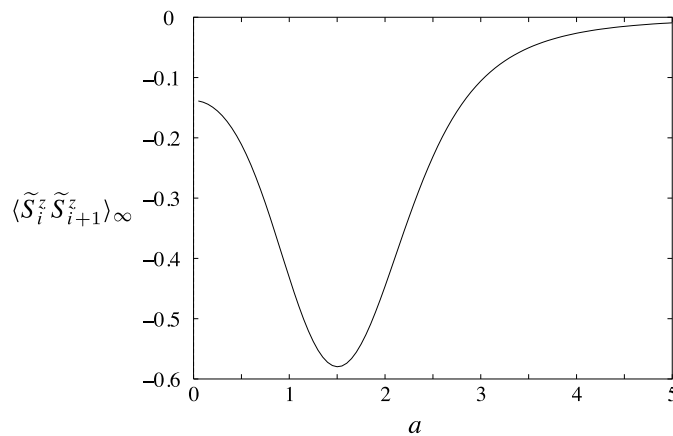


Figure 2. Correlation between adjacent rungs as a function of a .

The first two terms approach $-\frac{9}{4}$ in the Néel limit $a \rightarrow \infty$, but the last two terms converge to $+\frac{9}{4}$, since the spin operators act on the same sublattice. The minimum at $a \approx 1.5$ is very close to the maximum of the fluctuations (cf figure 1).

As a function of the distance r , the correlation between \tilde{S}_1^z and \tilde{S}_r^z decays exponentially, i.e. $\langle \tilde{S}_1^z \tilde{S}_r^z \rangle_\infty \propto \exp(-r/\xi_l)$. Figure 3 shows the a -dependence of the corresponding inverse correlation length ξ_l^{-1} . Note the divergence at $a = 1$. At this point, the weight of *all* non-vanishing vertices of the corresponding classical vertex model (cf the appendix) is 1. This corresponds to an infinite temperature, if the vertex weight is interpreted as a ‘Boltzmann weight’. The correlation length remains finite for all values of a , so the system is never critical.

For $a \neq 0$, the constructed optimum ground state $|\Psi_0\rangle$ on the ladder is the *only* ground state of the global Hamiltonian (1). The proof can be carried out by induction according to system size and is omitted here. In the special case $a = 0$, the global ground state degeneracy grows exponentially with system size.

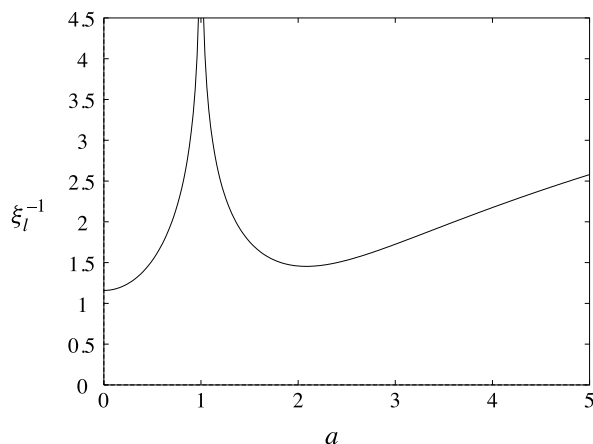


Figure 3. Inverse longitudinal correlation length as a function of a .

5. Summary and outlook

We have constructed an *optimum ground state* for a 5-parametric spin- $\frac{3}{2}$ model on the two-leg ladder. The Hamiltonian is completely homogeneous and contains only nearest-neighbour couplings. The local interaction operator exhibits S^z -conservation and parity invariance. No external magnetic field is applied. For special values of the parameters, the system has complete $SO(3)$ symmetry.

Optimum ground states are not only ground states of the global Hamiltonian, but also of every local interaction operator. For the present model, the ground state is given in terms of a *vertex state model*. A set of vertices, which have single-spin states as their values, is assigned to each lattice site. Concatenating these vertices on the two-leg ladder yields the global ground state. Vertex state models are straightforward generalizations of the well known *matrix product ground states* for spin-chains. The ground state contains a continuous parameter a and a discrete parameter $\sigma = \pm 1$.

Properties of the ground state have been calculated by using the transfer matrix technique. The sublattice magnetization and the total magnetization vanish, so the ground state is antiferromagnetic. Two-point correlations along the ladder decay exponentially. The fluctuations of the sublattice magnetization, the nearest-neighbour correlation, and the longitudinal correlation length have been determined as a function of the parameter a . As the correlation length is always finite, the system is never critical. Except for $a = 0$, the global ground state is unique.

For other spin- $\frac{3}{2}$ models on the two-leg ladder, e.g. with generic Heisenberg interaction, the constructed ground state could serve as a variational ground state. In this scenario, the anisotropy parameter a plays the role of a variational parameter. Optimum ground states can also be constructed for more sophisticated ladder models, e.g. with next-to-nearest-neighbour interaction and inhomogeneous couplings.

Appendix. The transfer matrix technique

Consider a local observable A_i , which acts on the spins on rung number i . Its expectation value in the ground state is defined as

$$\langle A_i \rangle_{\Psi_0} = \frac{\langle \Psi_0 | A_i | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}. \quad (\text{A.1})$$

The denominator can be interpreted as two identical vertex state models on top of each other. The upper (lower) one represents the bra- (ket-) vector. Since the vertices at a given lattice site generate only local spin states, the inner product can be taken separately at each lattice site. The result is a *classical* vertex model, i.e. the ‘weights’ of the vertices are numbers, but each vertex emanates *two* bonds in each direction. One set of bonds carries the arrow variables of the bra-vector, the other one carries those of the ket-vector. Therefore the inner product $\langle \Psi_0 | \Psi_0 \rangle$ can be constructed from the L -fold product of the *transfer matrix*

$$T_{(\mu_1, \mu_2, \nu_1, \nu_2)}^{(\mu_3, \mu_4, \nu_3, \nu_4)} = \frac{\mu_1 \quad \mu_3}{\nu_1 \quad \nu_3} \left| \begin{array}{c} \mu_1 \quad \mu_3 \\ \mu_2 \quad \mu_4 \\ \nu_2 \quad \nu_4 \end{array} \right| = \left\langle \begin{array}{c} \mu_1 \quad \mu_3 \\ \mu_2 \quad \mu_4 \\ \nu_1 \quad \nu_3 \\ \nu_2 \quad \nu_4 \end{array} \right\rangle. \quad (\text{A.2})$$

It has four incoming ($\mu_1, \mu_2, \nu_1, \nu_2$) and four outgoing indices ($\mu_3, \mu_4, \nu_3, \nu_4$). Each index represents a binary bond variable, so T is a 16×16 -matrix. As we are dealing with periodic boundary conditions, the trace must be used to obtain the inner product

$$\langle \Psi_0 | \Psi_0 \rangle = \text{tr} T^L. \quad (\text{A.3})$$

The numerator of (A.1) can also be interpreted as a classical vertex model. It differs from the one for the denominator only at rung number i , where the observable A_i acts nontrivially. Therefore the numerator also has a matrix product representation, but the i th factor is the *associated transfer matrix* $T(A)$ instead of T :

$$\langle \Psi_0 | A_i | \Psi_0 \rangle = \text{tr}[T^{i-1} T(A) T^{L-i}] = \text{tr}[T(A) T^{L-1}]. \quad (\text{A.4})$$

$T(A)$ is obtained from definition (A.2) by inserting A_i between the bra- and the ket-vector on the r.h.s. of the equation. Note that (A.4) is independent of i , as $|\Psi_0\rangle$ has perfect translational invariance. Since T is symmetric, its eigenvalues χ_k and its normalized eigenvectors $|u_k\rangle$ can be used to calculate the L -fold matrix products. This yields

$$\langle A_i \rangle_{\Psi_0} = \frac{\sum_k \langle u_k | T(A) | u_k \rangle \chi_k^{L-1}}{\sum_k \chi_k^L} \quad (\text{A.5})$$

for the expectation value of A_i . In the thermodynamic limit $L \rightarrow \infty$, which is the most interesting case, only the largest eigenvalue χ_{\max} survives. This simplifies (A.5) to

$$\langle A_i \rangle_{\infty} = \frac{\langle u_{\max} | T(A) | u_{\max} \rangle}{\chi_{\max}}. \quad (\text{A.6})$$

The above consideration can be easily extended to two-point correlation functions. In the thermodynamic limit the corresponding formula is

$$\langle A_1 B_r \rangle_{\infty} = \frac{1}{\chi_{\max}^2} \sum_k \langle u_{\max} | T(A) | u_k \rangle \langle u_k | T(B) | u_{\max} \rangle \left(\frac{\chi_k}{\chi_{\max}} \right)^{r-2}. \quad (\text{A.7})$$

If the following mapping of matrix indices to arrow configurations is used, the transfer matrix (A.2) takes a block-diagonal form:

index	upper bra μ_1/μ_3	upper ket ν_1/ν_3	lower bra μ_2/μ_4	lower ket ν_2/ν_4	
1	←	←	←	←	
2	→	→	→	→	
3	←	←	→	→	
4	→	→	←	←	
5	←	→	→	←	
6	→	←	←	→	
7	←	←	←	→	(A.8)
8	→	→	←	→	
9	←	→	←	←	
10	←	→	→	→	
11	←	←	→	←	
12	→	→	→	←	
13	→	←	←	←	
14	→	←	→	→	
15	←	→	←	→	
16	→	←	→	←	

The first block is the 6×6 -matrix

$$T_{1 \rightarrow 6} = \begin{pmatrix} 2 & 2a^2 & 1+a^2 & 1+a^2 & \sigma & \sigma \\ 2a^2 & 2 & 1+a^2 & 1+a^2 & \sigma & \sigma \\ 1+a^2 & 1+a^2 & 2 & 1+a^4 & \sigma & \sigma \\ 1+a^2 & 1+a^2 & 1+a^4 & 2 & \sigma & \sigma \\ \sigma & \sigma & \sigma & \sigma & 2 & 0 \\ \sigma & \sigma & \sigma & \sigma & 0 & 2 \end{pmatrix}. \quad (\text{A.9})$$

This submatrix contains the leading eigenvalue of the whole transfer matrix for all values of the parameters.

The 4×4 -blocks for indices $7 \rightarrow 10$ and $11 \rightarrow 14$ are identical. Both are given by

$$T_{7 \rightarrow 10} = T_{11 \rightarrow 14} = \begin{pmatrix} 2\sigma & \sigma(1+a^2) & 1 & 1 \\ \sigma(1+a^2) & 2\sigma & 1 & 1 \\ 1 & 1 & 2\sigma & \sigma(1+a^2) \\ 1 & 1 & \sigma(1+a^2) & 2\sigma \end{pmatrix}. \quad (\text{A.10})$$

The remaining two-dimensional subspace of indices 15 and 16 is already diagonal:

$$\chi_{15} = \chi_{16} = 2. \quad (\text{A.11})$$

Since both submatrices (A.9) and (A.10) are symmetric, an orthogonal eigenbasis of the complete transfer matrix exists. However, exact expressions for the eigensystem are very complicated, so they have been omitted.

Acknowledgment

This work was performed within the research program of the Sonderforschungsbereich 341, Köln-Aachen-Jülich.

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