Exact Groundstates for Antiferromagnetic Spin-One Chains with Nearest and Next-Nearest Neighbour Interactions

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We have found the exact ground state for a large class of antiferromagnetic spin-one chains with nearest and next-nearest neighbour interactions. The ground state is characterized as a matrix product of local site states and has the properties characteristic of the Haldane scenario.

1 Introduction

In recent years antiferromagnetic spin-one chains have been subject to intensive analytical, numerical and experimental investigations. Of main interest are groundstate phase diagrams and critical properties with respect to variations of interaction parameters resp. anisotropies of the systems. The study of anisotropy effects is quite important, as all experimental realizations indicate that quasi-one-dimensional systems have restricted symmetries [1-7].

In [8] we started the investigation of a most general class of spin-one chains with anisotropic nearest-neighbour exchange interactions and single ion anisotropy. In a large parameter subspace of this model the groundstates were found in the form of “matrix products”. The corresponding phase diagram consists of several parts which are separated by transition lines of first and second order. Away from these lines the model has a unique ground state, an energy gap to the excited states and exponential decay of ground state correlations. Thus, the so-called Haldane scenario was verified for the considered model. This scenario, conjectured in 1983 [9, 10] for

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certain isotropic models with integral spins, is quite interesting as it points out a striking difference between the behaviour of isotropic integral and half-integral spin chains. The latter are expected to have no gap and algebraic decay of correlations.

The first model for which the Haldane scenario was proven rigorously is the Valence-Bond-Solid (VBS) model — a spin-one chain with special isotropic bilinear and bi-quadratic nearest neighbour interactions \[11, 12\]. In a further development the unique VBS ground state was cast into a matrix product of single site states and generalized to anisotropic interactions \[13, 14\]. The concept of “matrix product ground states” (MPGs) was then applied to most general spin-one models \[8\]. The MPGs have non-trivial correlations and thus differ notably from the ground states of the Majumdar-Ghosh-type models \[15\].

In this paper we investigate the additional effects of interactions between next-nearest neighbours \[16\]. The anisotropies assumed in \[8\] for the local spin pair interactions will be retained.

## 2 Model

For realistic spin-one chains we assume the following symmetries:

- a) rotational invariance in the \((x, y)\)-plane,
- b) invariance under \(S^z \rightarrow -S^z\),
- c) local homogeneity of interactions, \(h_{j, j+1} = h_{j+1, j}\).

The most general anisotropic spin-one chain with nearest and next-nearest neighbour interactions can then be written in the following form:

\[
\mathcal{H} = \sum_{j=1}^{L} h_{j,j+1,j+2} = \sum_{j=1}^{L} \frac{1}{2}(h_{j,j+1} + h_{j+1,j+2}) + h_{j,j+2},
\]

\[
h_{j,j+1} = \alpha_0 A_j^2 + \alpha_1 (A_j B_j + B_j A_j) + \alpha_2 B_j^2 + \alpha_3 A_j + \alpha_4 B_j (1 + B_j) + \alpha_5 \left( (S_j^z)^2 + (S_{j+1}^z)^2 \right),
\]

\[
h_{j,j+2} = \tilde{\alpha}_0 \tilde{A}_j^2 + \tilde{\alpha}_1 (\tilde{A}_j \tilde{B}_j + \tilde{B}_j \tilde{A}_j) + \tilde{\alpha}_2 \tilde{B}_j^2 + \tilde{\alpha}_3 \tilde{A}_j + \tilde{\alpha}_4 \tilde{B}_j (1 + \tilde{B}_j) + \tilde{\alpha}_5 \left( (S_j^z)^2 + (S_{j+2}^z)^2 \right) + c,
\]

with real parameters \(\alpha_j\), \(\tilde{\alpha}_j\) and a constant \(c\). We impose periodic boundary conditions.

The nearest (next-nearest) neighbour interactions \(A_j\) and \(B_j\) (\(\tilde{A}_j\) and \(\tilde{B}_j\)) are defined
\[ A_j = S_j^+ S_{j+1}^+ = S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ \quad \text{(transverse)}, \quad (4) \]
\[ B_j = S_j^z S_{j+1}^z \quad \text{(longitudinal)}, \quad (5) \]
\[ \tilde{A}_j = S_j^+ S_{j+2}^+ = S_j^+ S_{j+2}^- + S_j^- S_{j+2}^+ \quad \text{(transverse)}, \quad (6) \]
\[ \tilde{B}_j = S_j^z S_{j+2}^z \quad \text{(longitudinal)}, \quad (7) \]

with \( S^\pm = (S^x \pm iS^y)/\sqrt{2} \). Thus we have a model with 12 non-trivial parameters \( \alpha_j, \tilde{\alpha}_j \), including a scale, and an additional constant \( c \).

If all the \( \tilde{\alpha}_j \)'s are equal to zero, we obtain the nearest neighbour model investigated in \[8\]. For this 6-parameter model it was shown that the exact ground state could be found as a unique MPG in a 4-dimensional parameter sub-space. For various reasons it is interesting to know what will happen if next-nearest neighbour interactions are considered. The question is for which interaction parameters the MPG ansatz is still applicable and what is the structure of the solution manifold.

3 Matrix product ground states

We shall be interested in the antiferromagnetic case of the model where the ground state is characterized by \( S_{\text{total}}^z = 0 \). We use the same ansatz as in \[8\] to determine the ground state in the form of a matrix product state.

Denoting the \( S_j^z \) eigenstates with eigenvalues 0 and ±1 by \( |0>_j \) and \( |\pm>_j \), we define at each site \( j \) a 2 × 2-matrix:

\[ g_j = \begin{pmatrix} |0>_j & -\sqrt{a}|+>_j \\ \sqrt{a}|-_j & -\sigma|0>_j \end{pmatrix} \quad (8) \]

with non-vanishing parameters \( a \) and \( \sigma \). The latter will turn out to be ±1. For the global ground state of (1) we use the ansatz

\[ |\psi_0 (a, \sigma) > = \text{Trace} (g_1 \otimes g_2 \otimes \ldots \otimes g_L), \quad (9) \]

where \( \otimes \) denotes a matrix multiplication of 2 × 2-matrices with a tensor product of the matrix elements \[8\].

By adjusting the constant \( c \), we guarantee the condition \( h_{j,j+1,j+2} \geq 0 \) (and thus \( \mathcal{H} \geq 0 \)). We demand the MPG (9) to be a ground state of (1) with eigenvalue 0:
$\mathcal{H}|\psi_0(a,\sigma)\rangle = 0$. This obviously is equivalent with $h_{j,j+1,j+2}|\psi_0(a,\sigma)\rangle = 0$. As (9) is a product state, it is sufficient to demand

$$h_{j,j+1,j+2}(g_j \otimes g_{j+1} \otimes g_{j+2}) = 0. \tag{10}$$

Equation (10) means that the local interaction $h_{j,j+1,j+2}$ acts upon all the four entries of the $g \otimes^3$ matrix. It can be shown that (10) requires nine linear equations for the parameters $\alpha_j$ and $\tilde{\alpha}_j$ which guarantee the ground state property of $|\psi_0(a,\sigma)\rangle$ under the condition $h_{j,j+1,j+2} \geq 0$. As we have $12 + 2 = 14$ parameters, namely the coupling parameters $\alpha_j$, $\tilde{\alpha}_j$ and the two parameters $a$ and $\sigma$ of the ansatz (9), this means that MPGs can be constructed in a five-dimensional parameter submanifold. The uniqueness of the ground state (9) is achieved by a strictly four-fold degenerate lowest eigenvalue zero of the local interaction $h_{j,j+1,j+2}$ [14]. This condition determines the geometrical structure of the five dimensional solution manifold.

4 Results

Explicit calculations show that (10) is satisfied under the following conditions

$$\begin{align*}
(0) \quad \sigma &= \text{sign} \alpha_3, \\
(i) \quad a(\alpha_0 + 2\tilde{\alpha}_3) &= \alpha_3 - \alpha_1, \\
(ii) \quad \alpha_2 &= \alpha_0 a^2 - 2|\alpha_3| + 4\tilde{\alpha}_3, \\
(iii) \quad \alpha_5 &= |\alpha_3| + \alpha_0(1 - a^2) - a^2\tilde{\alpha}_3, \\
(iv) \quad \tilde{\alpha}_0 &= -\alpha_3, \\
(v) \quad -a\sigma\tilde{\alpha}_0 &= \tilde{\alpha}_3 - \tilde{\alpha}_1, \\
(vi) \quad \tilde{\alpha}_2 &= (2 - a^2)\tilde{\alpha}_3, \\
(vii) \quad \tilde{\alpha}_5 &= \frac{1}{2}(a^2 - 4)\tilde{\alpha}_3, \\
(viii) \quad \tilde{\alpha}_4 &= \frac{1}{2}(a^2 - 2)\tilde{\alpha}_3.
\end{align*}$$

As pointed out before, the conditions (i) to (viii) define eight linear equations for the interaction parameters $\alpha_j$ and $\tilde{\alpha}_j$ whereas (0) specifies $\sigma$. The most striking effect is that the ansatz (9) imposes strict conditions upon the parameters for the next-nearest neighbour interactions, equations (iv) to (viii): As soon as $\tilde{\alpha}_3 \neq 0$, all the other parameters $\tilde{\alpha}_j$ do not vanish either, except for special values of the parameter $a$. In particular we find: $\tilde{\alpha}_0 \neq 0$. This means that as far as the next-nearest neighbour interactions are concerned biquadratic terms cannot be neglected.

As $\tilde{\alpha}_3$ approaches zero (limit of only nearest neighbour interactions), the equations (iv) to (viii) become irrelevant. Besides, the $\tilde{\alpha}_3$-terms in (i), (ii) and (iii) vanish.
Comparing the two situations, $\tilde{\alpha}_3 = 0$ and $\tilde{\alpha}_3 \neq 0$, the following observation can be made: Starting from a model with 12 non-trivial parameters for nearest and next-nearest neighbour interactions, we remain with five free parameters, $\tilde{\alpha}_3, \alpha_0, \alpha_3, \alpha_4$ and $a$, whereas for only nearest neighbour interactions ($\tilde{\alpha}_3 = 0$) we remain with four free parameters, $\alpha_0, \alpha_3, \alpha_4$ and $a$, on the basis of a model with 6 non-trivial interaction parameters.

The ground state property of (9) can be guaranteed under the condition $h \geq 0$. The uniqueness of (9) is valid if all the other eigenvalues of the local interaction are strictly positive. The diagonalization of $h_{j,j+1,j+2}$ yields a set of linear, quadratic and cubic inequalities for the parameters $\alpha_j$ and $\tilde{\alpha}_j$ (see the appendix and [16]). Those inequalities define a five-dimensional parameter manifold with a complex geometrical structure. In the limit $\tilde{\alpha}_j \to 0$ this manifold turns into the four-dimensional sub-space defined by the conditions $\alpha_0 > 0$, $\alpha_4 > 0$, $\alpha_3 \neq 0$ and $a \neq 0$. A detailed discussion of this solution manifold of the nearest neighbour model can be found in [8].

For general $\tilde{\alpha}_3 \neq 0$ there are the following most significant effects (see also the appendix and [16]):

We get a higher degree of freedom concerning the choice of the parameters $\alpha_0$ and $\alpha_4$, in particular they can be set equal to zero (A.1). On the other hand the ansatz (9) implies stricter conditions for the parameters $\alpha_3, \alpha_1$ and thus $a$: The parameter $|\alpha_3|$ must exceed a certain finite minimum value (A.2) in contrast to the simple condition: $|\alpha_3| \neq 0$ for $\tilde{\alpha}_3 = 0$. As in [8] the parameter $a$ must satisfy the condition $a \neq 0$. But in contrast to [8], depending on the choice of the values for $\alpha_0$ and $\alpha_4$, $a$ must no longer be chosen arbitrarily small or large (A.2, A.5).

The ground state correlation functions can be calculated, using the transfer matrix method of [14, 8]. In the thermodynamic limit $L \to \infty$ and for $r \geq 2$ we obtain the same longitudinal and transverse 2-site correlation functions with exponential decay as in [8]:

$$<S_1^z S_r^z> = -\frac{a^2}{(1 - |a|)^2} \left(\frac{1 - |a|}{1 + |a|}\right)^r = -\frac{a^2}{(1 - |a|)^2} e^{-\frac{r}{\xi_l}}$$

(11)

with the longitudinal correlation length:

$$\frac{1}{\xi_l} = \ln \left|\frac{1 + |a|}{1 - |a|}\right|,$$

(12)
\[
\langle S^x_1 S^x_r \rangle \equiv \langle S^y_1 S^y_r \rangle = -|a| (\sigma + \text{sign}a) \left( \frac{-\sigma}{1 + |a|} \right)^r
\]

(13)

with the transverse correlation length

\[
\frac{1}{\xi_t} = \ln |1 + |a||.
\]

(14)

As the correlation functions depend on the overlap parameter \(a\), the only difference between the cases \(\tilde{\alpha}_3 = 0\) and \(\tilde{\alpha}_3 \neq 0\) is given by equation (i) which describes the functional dependence of \(a\) on the interaction parameters.

Note that for \(a \to 0\) there is a critical transition (diverging correlation lengths (12),(14)) into a phase where all the spins lie in the \(xy\)-plane: \(|\psi_0\rangle \to |0000\ldots>\).

For \(a \to \infty\) the MPG approaches the Néel states \(|\pm \mp \pm \pm \ldots>\).

There is a finite gap to the excitations in the thermodynamic limit. This can be understood using the same arguments as in [8]. The MPG ansatz generates a "Haldane scenario" in a natural way. The global ground state of (1) is composed of local ground states in a way which is independent of the system’s size. For this reason the properties of the finite system, especially the energy gap, persist in the thermodynamic limit \(L \to \infty\).
Appendix

The diagonalization of $h_{j,j+1,j+2}$ yields the following conditions for the uniqueness of the MPG (9):

\[
\begin{align*}
\alpha_4 + \min(\tilde{\alpha}_3, \frac{1}{2}|\alpha_3|) &> 0, \\
\tilde{\alpha}_3 + \frac{1}{2}|\alpha_3| &> 0, \\
\alpha_0 + \frac{1}{2}|\alpha_3| &> 0, \\
|\alpha_3| &> 0, \\
2a^2\tilde{\alpha}_3 + 2\alpha_4 + 3|\alpha_3| &> 0, \\
\tilde{\alpha}_3(2(a^2 - 2)(2\tilde{\alpha}_3 + \alpha_4) + |\alpha_3|(a^2 + 2)) + 2\alpha_4|\alpha_3| &> 0, \\
2\alpha_0(1 + a^2) + 2a^2\tilde{\alpha}_3 + 3|\alpha_3| &> 0, \\
|\alpha_3|(\tilde{\alpha}_3 + \alpha_0) - 2\tilde{\alpha}_3(2\tilde{\alpha}_3 + \alpha_0) &> 0.
\end{align*}
\] (A.1)

Using the following abbreviations:

\[
\begin{align*}
d_1 & = 2(\tilde{\alpha}_3 + \alpha_4), \\
d_2 & = \alpha_4 + \frac{1}{2}|\alpha_3| + \tilde{\alpha}_3, \\
d_3 & = \tilde{\alpha}_3(3 - a^2) + \frac{1}{2}\alpha_0 + \alpha_4, \\
d_4 & = |\alpha_3| + \tilde{\alpha}_3(a^2 - 2), \\
d_5 & = \frac{1}{2}(|\alpha_3| + a^2\alpha_0) + \tilde{\alpha}_3(a^2 - 1), \\
d_6 & = |\alpha_3| - \tilde{\alpha}_3, \\
d_7 & = \alpha_0 + 2\tilde{\alpha}_3, \\
d_8 & = \frac{1}{2}(\alpha_0 + |\alpha_3|) + \tilde{\alpha}_3 \\
d_9 & = |\alpha_3|, \\
d_{10} & = a^2(\alpha_0 + \tilde{\alpha}_3), \\
n_1 & = \frac{1}{2}\alpha_0, \\
n_2 & = \frac{1}{2}\alpha_3, \\
n_3 & = \frac{1}{2}(\alpha_3 - \alpha_1), \\
n_4 & = -\tilde{\alpha}_3, \\
n_5 & = \tilde{\alpha}_3, \\
n_6 & = a\sigma\tilde{\alpha}_3, \\
\end{align*}
\] (A.3)
we further obtain:
\[\begin{align*}
&d_3 + d_5 > 0, \\
&(d_3 + n_5)(d_5 - n_5) - n_3^2 > 0, \\
&d_3 + d_5 + d_7 + d_9 > 0, \\
&(d_3 + d_5)(d_7 + d_9) + d_3d_5 + d_7d_9 \\
&\quad + n_5(d_3 - d_5 - n_5) - 2(n_1^2 + n_2^2 + n_6^2) - 3n_3^2 > 0, \\
&d_3(d_5 + n_5)(d_7 + d_9) + d_7d_9(d_3 + d_5) \\
&\quad + n_3^2(4n_1 + 2n_5) + 4n_2n_3n_6 \\
&\quad - 2n_1^2(d_5 + d_9) - 2n_2^2(d_3 + d_7) - n_3^2(2d_3 + d_7 + 3d_9) \\
&\quad - n_5(d_7 + d_9)(d_5 + n_5) - 2n_6^2(d_5 + d_7 + n_5) + 2n_5(n_2^2 - n_1^2) > 0.
\end{align*}\]

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