Exact trimer ground states on a spin-1 chain(*)

J. Sólyom(**) and J. Zittartz(***)

1 Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O.Box 49, Hungary
2 Institut für Theoretische Physik, Universität zu Köln, Zülpicherstr. 77, 50937 Köln, Germany

(received ; accepted )

PACS. 75.10.Jm– Quantized spin models.

Abstract. – We construct a new spin-1 model on a chain. Its ground state is determined exactly which is three-fold degenerate by breaking translational invariance. Thus we have trimerization. Excited states cannot be obtained exactly, but we determine a few low-lying ones by using trial states, among them solitons.

Spin chains and spin ladders have been intensively studied in recent years [1]. Besides the Bethe ansatz solvable models there is an increasing number of models where at least the ground state is known exactly and where eventually the gap to the first excited state can be calculated [2]. Typically in the ground state of these models the correlations are of short range which implies a finite gap. One natural way to construct such models in one dimension is to use the matrix product method [3] which is based on the concept of “optimum ground states” as explained in ref. [4].

In some cases translational symmetry is spontaneously broken leading to twofold degenerate, dimerized ground states. To the best knowledge of the authors no model has been found so far where the ground state would be threefold degenerate, thus leading to trimerization. For the first time we construct such a model.

There exists one model, the Uimin-Lai-Sutherland (ULS) model [5], which is a special case of the spin-1 bilinear-biquadratic chain, where the excitation spectrum has a tripled periodicity in the Brillouin zone, namely soft modes appear at \( q = 0 \) and \( q = \pm 2\pi/3 \), however, the ground state itself does not break translational symmetry.

For later convenience the Hamiltonian of the spin-1 bilinear-biquadratic model is written

(*) Work performed within the research program of the Sonderforschungsbereich 341, Köln-Aachen-Jülich
(**) E-mail: solyom@mail.szfki.kfki.hu
(***E-mail: zitt@thp.uni-koeln.de

Typeset using EURO-TpX
in the form

\[ H = \sum_{i=1}^{N} \left( (S_i \cdot S_{i+1})^2 + \alpha (S_i \cdot S_{i+1}) \right). \] (1)

The ULS point corresponds to \( \alpha = 1 \). For \( \alpha > 1 \) a gap opens up in the excitation spectrum above the unique ground state, if the chain is periodically closed. At \( \alpha = 3 \) we get the AKLT model \(^{(1)}\), where the existence of the gap has been proven. For \( \alpha < 1 \) the gapless spectrum with three soft modes presumably survives \(^{(2)}\). Since a gapless spectrum and, correspondingly, power law like decaying correlations should be an exception, and generically a spin chain should have a finite gap, one might expect to find a gapped trimerized state by perturbing away from the Hamiltonian given above.

To construct such a model that has an exact threefold degenerate ground state with a finite gap to the excitations we observe that the quantity

\[ A_{i,j} = (S_i \cdot S_j)^2 + \alpha (S_i \cdot S_j) + \alpha - 1 \] (2)

has the following properties. As eigenstates arrange in multiplets, we denote the 2-spin singlet state at site \( i \) and \( j \) by \( s[i,j] \), and similarly by \( t[i,j] \) and \( q[i,j] \) the triplet and quintuplet states. Then we find

\[ A_{i,j} \begin{pmatrix} s[i,j] \\ t[i,j] \\ q[i,j] \end{pmatrix} = \begin{cases} (3 - \alpha) s[i,j] \\ 0 t[i,j] \\ 2\alpha q[i,j] \end{cases}. \] (3)

This implies that the triplet has the lowest energy in the range \( 0 < \alpha < 3 \).

For three spins at sites \( i, j, k \) one has one septuplet, two quintuplets, three triplets, and precisely one totally antisymmetric singlet. This trimer singlet is given by

\[ S[i,j,k] = \frac{1}{\sqrt{6}} [(+,0,-) + (0,-,+) + (-,+0) - (-,0,+) + (0,+,-) - (+,-,0)] \] (4)

in terms of the three states \((+), (-)\) and \((0)\) of a spin-1 operator. Then using the fact that in order to form a singlet with the third spin, any two spins have to form a triplet, one gets easily from eq. \((1)\)

\[ A_{i,j} S[i,j,k] = A_{i,k} S[i,j,k] = A_{j,k} S[i,j,k] = 0. \] (5)

Using this property one sees immediately that the Hamiltonian

\[ H = \sum_{i=1}^{N} h_{i,i+1,i+2,i+3} = \sum_{i=1}^{N} A_{i,i+2} A_{i+1,i+3} \] (6)

has precisely three zero energy ground states. For a finite periodically closed chain of \( N = 3p \) sites, where \( p \) is an integer, these three states are:

\[ \Psi_1 = \prod_{i=1}^{p} S[3i - 2, 3i, 3i + 2], \]
\[ \Psi_2 = \prod_{i=1}^{p} S[3i - 1, 3i + 1, 3i + 3], \]
\[ \Psi_3 = \prod_{i=1}^{p} S[3i, 3i + 2, 3i + 4]. \] (7)
They are ground states, as $\mathcal{H}$ and $h$ of eq. (6) are positive-semidefinite in $0 < \alpha < 3$, and they are optimum ground states, as in the sense of ref. [4] they are simultaneously ground states of all local interactions $h$. For a finite system these states are not strictly orthogonal, but their overlap goes to zero exponentially with $N \to \infty$ namely as $\gamma^N (0 < \gamma < 1)$.

To visualize the states we show one of them in fig. 1 by connecting the sites belonging to the trimer singlets by valence bonds. Because the trimer singlet is antisymmetric under left to right reflection, i.e., $[i,j,k] \to [k,j,i]$, the bonds have to be directed. It is more convenient to draw the chain as a zig-zag ladder which is shown in fig. 2. When $N = 6p$, this is a genuine ladder, while when $N = 3(2p + 1)$, it can be thought of as part of a Moebius ribbon. In what follows we will use everywhere this zig-zag ladder representation.

![Fig. 1. – Valence bond representation of the ground state.](image1)

![Fig. 2. – The ground state configuration represented on a zig-zag ladder.](image2)

That these states are in fact the ground states of the Hamiltonian in the range $0 < \alpha < 3$, follows immediately from eq. (3). At $\alpha = 0$ the quintuplet of the spins at site $i$ and $j$ has the same energy as the singlet, so at this point the degeneracy of the ground state becomes exponentially large. For $\alpha < 0$ the quintuplet has the lowest energy, leading to the fully polarized ferromagnetic state. The transition of the trimer phase to the ferromagnetic one is of first order.

At $\alpha = 3$ the 2-spin singlet and triplet local pairs become degenerate, producing again an exponentially large degeneracy, while for $\alpha > 3$ we get to the massive, Haldane-like regime with unique ground state.

Next we discuss excited states of the model. They cannot be calculated exactly, but clearly there has to be a gap to the excitations, because the ground state is formed of short range valence bonds. The simplest excited state could be a state where one trimer singlet is broken up and is replaced by a triplet (Tri), quintuplet (Quint) or septuplet (Sept) of the three spins, e.g.,

$$\Phi_B(l) = B[3l - 2, 3l, 3l + 2] \prod_{i \neq l} S[3i - 2, 3i, 3i + 2],$$

(8)

where $B$ stands for Tri, Quint or Sept. Using these as trial states and calculating their energy as the average $E = \langle H \rangle$, we see that two terms of the Hamiltonian give a non-zero contribution:

$$A_{3l-2,3l} A_{3l-1,3l+1} + A_{3l-1,3l+1} A_{3l,3l+2}.$$

(9)

As can be easily seen the Hamiltonian has no matrix element between states where different trimers are broken, and there is no overlap between these states. Therefore these excited states
have no dispersion. For the three possible triplet states we get the energy

\[
E_{\text{Tri}} = \begin{cases} 
(2 + \alpha)(\frac{1}{3} + \alpha), \\
(3 - a_1 - \alpha)(\frac{1}{3} + \alpha), \\
(3 - a_2 - \alpha)(\frac{1}{3} + \alpha),
\end{cases}
\] (10)

where \(a_{1,2}\) are the solutions of the equation

\[
a_{1,2} = 1 - \frac{3}{2}\alpha \pm \sqrt{(1 - \frac{3}{2}\alpha)^2 + 3 - \alpha}.
\] (11)

For the two quintuplet states the energies are

\[
E_{\text{Quint}} = \begin{cases} 
\alpha(\frac{1}{3} + \alpha), \\
3\alpha(\frac{1}{3} + \alpha),
\end{cases}
\] (12)

while for the septuplet state \(E_{\text{Sept}} = 4\alpha(1/3 + \alpha)\). One checks that the triplet gap with \(a_1\) in eq. (10) and the first quintuplet gap in eq. (12) are the lowest ones.

The lowest energy propagating modes are probably solitonic excitations, which are moving domain walls between two different ground states. In a ring of length \(N = 3p\), where the lattice spacing is taken to be unity, a soliton cannot appear alone. In the simplest case one needs three solitons to satisfy the periodic boundary condition. However, provided the chain is long enough, solitons can be studied separately assuming that the two ends are in different ground states.

A domain wall that perturbs the system as little as possible can be obtained on a chain of \(3p + 2\) sites between state \(\Psi_1\) on the left hand side and \(\Psi_3\) on the right hand side by having the spins at sites \(3l - 2\) and \(3l + 1\) forming a singlet, triplet or quintuplet, while all other spins are in their trimer singlet ground state. Similar domain walls appear between state \(\Psi_2\) on the left and \(\Psi_1\) on the right or \(\Psi_3\) on the left and \(\Psi_2\) on the right.

Such a state can be written as

\[
\Phi_c(l) = \prod_{i=1}^{l-1} S[3i - 2, 3i, 3i + 2] c[3l - 2, 3l + 1] \prod_{j=l}^{p} S[3j, 3j + 2, 3j + 4],
\] (13)

where \(c\) stands for \(s\), \(t\) or \(q\). It is shown in fig. 3.

Fig. 3. – Domain wall on a chain with \(3p + 2\) sites represented on a zig-zag ladder.

Only one term in the Hamiltonian will give a non-zero contribution to the energy, namely

\[
A_{3l-2,3l}A_{3l-1,3l+1}.
\] (14)

Although the Hamiltonian has no matrix element between states with different site index \(l\), a propagating mode is obtained since there is a finite overlap between these states. Now looking
for the moving soliton in the form
\[ \Phi_c(q) = \sum_{l=1}^{P} e^{i3ql} \Phi_c(l), \] (15)
we find for the energy of the singlet and quintuplet excitations
\[ E_{s,q}(q) = \frac{1}{4} \left( \frac{4}{3} + \alpha \right)^2 \left[ 5 - 3 \cos 3q \right], \] (16)
and
\[ E_{t,q}(q) = \frac{1}{4} \left( \frac{4}{3} + \alpha \right)^2 \left[ 5 + 3 \cos 3q \right] \] (17)
for the triplet excitations.

A somewhat more complicated domain wall is shown in fig. 4 between state \( \Psi_1 \) on the left and state \( \Psi_3 \) on the right. Because of its symmetric shape, the Hamiltonian has finite matrix elements between domain walls on different sites, giving direct propagation. In addition to that the overlap has also to be considered, giving finally a rather complicated dispersion relation. When the two spins form a singlet, the dispersion relation of the soliton is:
\[ E_{s}(q) = \frac{2}{9} \left[ (1 + 3\alpha)^2 + (1 - 2\alpha)^2 \cos 3q \right] \frac{5 - 3 \cos 3q}{14/3 - 2 \cos 3q}, \] (18)
while for the triplet
\[ E_{t}(q) = 2 \left( \frac{4}{3} + \alpha \right)^2 \left[ 1 + \frac{1}{4} \cos 3q \right] \frac{5 + 3 \cos 3q}{16/3 + 4 \cos 3q}, \] (19)
and for the quintuplet
\[ E_{q}(q) = \frac{2}{9} \left[ (1 + 3\alpha)^2 + \frac{1}{4} (1 + \alpha)^2 \cos 3q \right] \frac{5 - 3 \cos 3q}{14/3 - 2 \cos 3q}. \] (20)

It is interesting to speculate what happens if the model presented in this paper is perturbed away from the form given in eq. (6). As mentioned earlier both at \( \alpha = 0 \) and \( \alpha = 3 \) the degeneracy of the ground state gets exponentially large. Beyond these points the system becomes ferromagnetic, or a first order phase transition to a massive Haldane phase occurs. If extra parameters are introduced by making the couplings of the two-spin and four-spin terms independent, the trimerized phase will survive because of its finite gap. However, at some point the two legs of the zig-zag ladder become decoupled, and other phases may appear.

Finally we mention that the model can easily be generalized without changing essential properties. Namely for \( N = 6p \) one can have different parameters \( \alpha \) and \( \beta \) in the operators \( A \) acting on the upper and the lower legs, respectively. We like to thank Dr. A. Schadschneider for this hint.
Furthermore we mention that we have found other model Hamiltonians with trimer ground states. However, in all these cases they are degenerate with other ground states and the degeneracy is exponentially large. Clearly they are not so interesting.

***

One of the authors (J. S.) is grateful to the University of Cologne for the hospitality during his visit, where most of this work was done. The authors acknowledge the financial support of the Deutsche Forschungsgemeinschaft. The work was partially supported by the Hungarian Research Fund (OTKA) grant No. 30173.

REFERENCES

[1] For a review see Dagotto E., cond-mat/9908250 Preprint, (1999).
[2] For a review see Kolezhuk A. K. and Mišeska H.-J., Int. J. Mod. Phys. B, 12 (1998) 2325.
[3] Kl"umper A., Schadschneider A. and Zittartz J., J. Phys. A, 24 (1991) L955; Europhys. Lett., 24 (1993) 293.
[4] Niggemann H. and Zittartz J., Z. Phys. B, 101 (1996) 289.
[5] Uimin G. V., JETP Lett., 12 (1970) 225; Lai C. K., J. Math. Phys., 15 (1974) 1675; Sutherland B., Phys. Rev. B, 12 (1975) 3795.
[6] Affleck I., Kennedy T., Lieb E. H. and Tasaki H., Phys. Rev. Lett., 59 (1987) 799; Commun. Math. Phys., 115 (1988) 477.
[7] Fáth G. and Sólyom J., Phys. Rev. B, 44 (1991) 11836.
[8] Itoi C. and Kato M.-H., Phys. Rev. B, 55 (1997) 8295.