Exact ground states of spin-2 chains

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Abstract. – We use the matrix product approach to construct all optimum ground states of general anisotropic spin-2 chains with nearest-neighbour interactions and common symmetries. These states are exact ground states of the model and their properties depend on up to three parameters. We find three different antiferromagnetic Haldane phases, one weak antiferromagnetic and one weak ferromagnetic phase. The antiferromagnetic phases can be described as spin liquids with exponentially decaying correlation functions. The variety of phases found with the matrix product ansatz also gives insight into the behaviour of spin chains with arbitrary higher spins.

Introduction. – Haldane’s conjecture \([1,2]\) about the fundamental difference between integer and half-odd-integer spin chains has triggered a strong interest in low-dimensional systems with arbitrary spin \(S\), both theoretically and experimentally. New materials have been found which can be considered as realizations of spin chains with \(S > \frac{1}{2}\). For low-dimensional models mean-field theories are usually not very reliable due to the importance of quantum fluctuations. Therefore, exact results become very important. They allow to explore possible phases and study their properties. Since only few models are solvable exactly, \(e.g.\) by Bethe ansatz \([3]\), it is necessary to reach out for alternative methods. Next to numerical procedures like DMRG \([4,5]\) powerful analytical approaches are available. In this paper we use the idea of optimum ground states \([6–8]\) which allows to construct systematically \textit{exact} ground states. The method is not restricted to one-dimensional spin systems, but can also be generalized to construct ground states for quantum spin systems in arbitrary dimensions \([9,10]\), Hubbard models \([7]\) or stochastic processes \([11]\).

A prominent example for a spin-2 chain is \((2, 2'-bipyridine)trichloromanganese(III)\), where the spin-2 is carried by \(\text{Mn}^{3+}\) and the magnetic interaction by the Mn-Cl-Mn orbital overlap. Experiments by Granroth \textit{et al.} \([12]\) show antiferromagnetic behaviour with exponentially decaying correlation functions. In the present letter we will construct states which exhibit exactly this behaviour with a non-degenerate ground state. Not only antiferromagnetic phases can be realized for a spin-2 chain, but also weak antiferromagnetic and weak ferromagnetic ones. As the method of optimum ground states allows us to calculate ground-state expectation values and properties for these states, it provides a good overview over the large variety of phases encountered in spin-2 chains and their properties.

In the following we consider quantum spin chains described by a translational invariant Hamiltonian \(H = \sum_{(i,j)} h_{ij}\) with nearest-neighbour interactions \(h_{ij}\). 

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Definition. A global ground state $|\Psi_0\rangle$ is called optimum ground state (OGS) of $H = \sum_{(i,j)} h_{ij}$, if the global ground-state energy $E_0$ is just the sum of the local ground-state energy values $\epsilon_0$ of the local Hamiltonians $h_{ij}$.

In other words: If the local ground-state conditions $h_{ij} |\Psi_0\rangle = 0$ are complied (which can be achieved by adding the constant $-\epsilon_0$ to the local interaction $h_{ij}$), this yields the equivalence

$$H |\Psi_0\rangle = 0 \iff h_{ij} |\Psi_0\rangle = 0, \quad \forall i, j,$$  \hspace{1cm} (1)

since then 0 is a lower bound for $E_0$. The r.h.s. of (1) can be used as local conditions for the existence of an optimum ground state and its realization in terms of a matrix product ground state (MPG) (see below). Obviously, OGS are states without finite-size corrections. In [6,13,14] the matrix product ground-state approach has been described in more detail.

For the spin-1 chain [6] it is possible to construct one type of matrix product ground state for a Hamiltonian with the three symmetries: 1) rotational invariance in the ($x,y$)-plane, 2) spin flip invariance, 3) translation and parity invariance. In the case of spin-2 chains with these symmetries and nearest-neighbour interaction we find five different non-trivial MPGs. It can be understood easily that there exist no more than these five MPG, except for exponentially degenerate ones [15].

Usually, it is most common to find exact or approximate ground states or even the full spectrum for a given Hamiltonian. The modus operandi we use here is the other way round. First, we construct the optimum ground states for a given system and then we determine the subspace of Hamiltonians for which these are the ground states. Describing the local Hamiltonians $h_{ij}$ in terms of local eigenstates $|v_k\rangle$ of $\hat{S}_z^i + \hat{S}_z^{i+1}$ (eigenvalue $s$) and the parity operator $\hat{P}_{ij}$ (eigenvalue $p$) and the spin flip invariance lead to $h_{ij} = \sum_k \lambda_k |v_k\rangle\langle v_k|$ (see [16]).

For some sets of quantum numbers $s, p$ the $|v_k\rangle$ are not determined completely by the imposed symmetries. Additional superposition parameters control the “orientation” of the basis states $|v_k\rangle$ in their respective subspace. Requiring that a given OGS is an exact ground state of $H$ leads to restrictions on the $\lambda_k$ and the superposition parameters of the $|v_k\rangle$. For a spin-2 system with nearest-neighbour interaction and above-mentioned symmetries the total number of parameters is 22 [10]. Two parameters, the energy off-set and a scale, are trivial, which leads effectively to a 20 parameter model. For the most general model there are 25 local energy eigenstates.

As expected, such a model with 20 parameters in general has very complicated ground states of the global Hamiltonian $H$. The concept of optimum ground states and its realization through MPG yield a class of structural simple states. For these it is possible to calculate ground-state expectation values for arbitrary operators. The isotropic valence-bond-solid (VBS) model [17] emerges as a special case and the properties of this model turn out to be generic for a more general subspace of the 20 parameter space.

The matrix product ground state. – Following the procedure explained in [6], one can define several matrices which are suited for constructing matrix product ground states of the spin-2 chain. Such a matrix consists of single-spin states at site $i$ as its elements and the product of two such matrices is defined as a matrix product with the tensor product $\otimes$ for the spin states,

$$(m^{(i)} \cdot m^{(i+1)})_{\mu\nu} = \sum_k m^{(i)}_{\mu k} \otimes m^{(i+1)}_{k\nu}. \hspace{1cm} (2)$$

Definition. A matrix product ground state (MPG) is a global ground state of a spin chain of length $L$, which for periodic boundary conditions can be written in the form

$$|\Psi_0\rangle = \text{tr} \left( m^{(1)} \cdot m^{(2)} \cdot m^{(3)} \cdots m^{(L)} \right), \hspace{1cm} (3)$$
where $\text{tr}$ stands for “trace over the matrix space”, i.e. \( \sum_{\mu} (m^{(1)} \cdot m^{(2)} \cdots m^{(L)})_{\mu \nu} \). For a MPG to satisfy the above optimum ground-state condition, \( h_{i,i+1} |\Psi_0\rangle = 0 \) must hold for all \( i \). Due to the product structure of the ground state \( |\Psi_0\rangle \) this reduces to

\[
h_{i,i+1} (m^{(i)} \cdot m^{(i+1)})_{\mu \nu} = 0 \quad \text{for all } i, \mu, \nu. \tag{4}\]

This implies that each element of the product matrix \( (m^{(i)} \cdot m^{(i+1)}) \) is a local ground state (of \( h_{i,i+1} \)). These conditions lead to several restrictions on the parameters from the most general model. So the matrix product ground state becomes a global ground state of the specified parameter subspace. The MPG itself turns out to depend on up to three parameters.

To calculate expectation values and other physical properties a transfer matrix approach [14] can be used. Results thus obtained are presented in the following sections.

**MPGs on the spin-2 chain.** – We have investigated systematically matrix product states on a spin-2 chain with unique or finitely degenerate ground states and periodic boundary conditions. We found five MPGs with non-trivial product structure and different properties. In the following only the most significant properties will be presented. A more complete account will be published elsewhere [15].

**Haldane-antiferromagnet-A.** – The first MPG is defined by the homogeneous product

\[
|\Psi_0\rangle (a, x, \gamma) = \text{tr} \left( \prod_{i} m^{(i)} \right)
\]

This representation with three continuous, real parameters \( a, x, \gamma \) uses the canonical spin-2 basis states, i.e. the eigenstates of the \( S^z \)-operator \( \hat{S}_i^z |s^z\rangle_i = s^z |s^z\rangle_i \) and \( \hat{S}_i^z |\overline{s}^z\rangle_i = -s^z |\overline{s}^z\rangle_i \) at site \( i \). Since all \( h_{i,i+1} \) should be the same (for all \( i \)), we have to solve (4) for one arbitrary \( i \) only. These conditions lead to a 12-parameter subspace and an additional trivial parameter for the scale. In general inequalities must hold for these parameters. For more details see [15]. This parameter space includes the isotropic point. The ground state itself depends on the three parameters \( a, x, \gamma \) and is unique, which can be proven rigorously by complete induction [16].

The corresponding Hamiltonian can be written as the sum of the projection operators onto the \( S^z = 3 \) and \( S^z = 4 \) multiplets. For any other set of parameters the model has an anisotropy along the \( z \)-axis. However, in any case the ground state is unique as long as \( a \neq 0 \). For \( a = 0 \) the matrix product ansatz (MPA) is not unique; the degeneracy grows with system size as \( 3^L \). This case is not considered in the following.

The ground state defined by (5) is antiferromagnetic in the sense that all single-site magnetisations vanish: \( \langle \hat{S}^z \rangle \equiv \langle \hat{S}^x \rangle \equiv \langle \hat{S}^y \rangle \equiv 0 \). It follows that the square of the fluctuation is simply given by

\[
(\Delta S^z)^2 = \langle (\hat{S}^z)^2 \rangle - \langle \hat{S}^z \rangle^2 = \langle (\hat{S}^z)^2 \rangle \in [0, 4]. \tag{6}\]

The maximum \( (\Delta S^z)^2 = 4 \) is reached in the limit \( |a| \to \infty \) and \( \Delta S^z = 0 \) for \( |\gamma| \to \infty \). In the latter case the dominant contribution is proportional to \( \gamma^L |000 \cdots 0\rangle \). The 2-site correlation functions decay exponentially to zero. The longitudinal correlation function is given by

\[
\langle \hat{S}_i^z \hat{S}_r^z \rangle = \langle \hat{S}_i^1 \hat{S}_r^2 \rangle (\text{sign} (1 - a^2))^r e^{-(r-2)/\xi_i} \quad (r \geq 2), \tag{7}\]
Fig. 1 – Longitudinal (thin line) and transversal correlation length $\xi$ for $x = -3$ and $\gamma = -2$. This special choice of parameter values includes the isotropic point for $a = \sqrt{6}$ where the correlation lengths are equal.

Fig. 2 – For $x = 0$, $\gamma = 1$ the correlation lengths diverge in the limit $a \to 0$. Note that the crossing point does not correspond to an isotropic Hamiltonian.

with the longitudinal correlation

$$\xi_l^{-1} = \ln \left| \frac{\lambda}{1 - a^2} \right|, \quad \lambda = \frac{1}{2} \left( (1 + a^2 + \gamma^2) + \sqrt{(1 + a^2 - \gamma)^2 + 8x^2} \right).$$

(8)

The first part of the function is the expectation value of the nearest-neighbour correlation which is antiferromagnetic ($\langle \hat{S}_1^z \hat{S}_2^z \rangle \leq 0$) and varies from 0 (for $\gamma \to \infty$) to $-4$ (for $a^2 \to \infty$) [16]. For large $a$, the correlation function alternates in $r$ as an easy axis anisotropy is observed. The transversal correlation function decays exponentially, too,

$$\langle \hat{S}_x^\tau \hat{S}_r^\tau \rangle = \langle \hat{S}_1^x \hat{S}_r^x \rangle (|x| + \gamma)^r e^{-(r-2)/\xi_t}, \quad \xi_t^{-1} = \ln \left| \frac{\lambda}{|x| + \gamma} \right|.$$  

(9)

Both correlation lengths $\xi_l$ and $\xi_t$ are finite (except for $a = x = 0$, see fig. 2) and so the model is non-critical. The $a$-dependence (see figs. 1 and 2) looks quite similar to the spin-1 MPG correlation lengths presented in [6]. For large $a$, the anisotropy is of easy-axis type with $\xi_l > \xi_t$, whereas for small $a$ it is of easy-plane type. Indeed, this MPG is the analogue of the matrix product ground state of the spin-1 chain, e.g. the isotropic point (see fig. 1) is included in this phase for both spin chains. For both chains the antiferromagnetic phases (including the two antiferromagnetic ones described in the next subsections) are Haldane phases with 1) a unique ground state, 2) exponentially decaying correlation functions, and 3) a gap to the first excited state. Here we only have shown 1) and 2) of this scenario, but the existence of a gap can be shown along the lines of the proof outlined in [17].

**Haldane-antiferromagnet-B.** – Differently from the spin-1 chain, it is possible to construct further matrix product ground states for the spin-2 case. A simple one is a homogeneous product of matrices

$$m = \left( \begin{array}{cc} 0 & \sqrt{a} \sigma^1 \\ \sqrt{a} \sigma^0 & 1 \end{array} \right), \quad a \in \mathbb{R}, \quad \sigma \pm 1,$$

(10)

which, in contrast to the Haldane-antiferromagnet-A, depends on one continuous parameter $a$ and one discrete parameter $\sigma$. The state $|\Psi_0\rangle(a) = \text{tr} \left( \prod_i^L m_i \right)$ looks quite similar to the one
presented in [6] for the spin-1 case. Again, it can be shown that it is a unique ground state of $H$ in the appropriate subspace. Even the expectation values of all combinations of the $\hat{S}_i^z$ operators look the same as in the spin-1 case, only expectation values of $\hat{S}_i^+\hat{S}_j^-$ or $\hat{S}_i^-\hat{S}_j^+$ operators vary by a factor. The properties of this phase are much the same of the one before and so we report some expectation values only. The single-site magnetisations vanish and the square of the fluctuation just as the longitudinal correlations function are the same as the ones for the spin-1 chain [6]. Differently from the spin-1 chain, the transversal correlation function reads

$$\langle \hat{S}_i^x \hat{S}_j^x \rangle = -3|a|(\text{sign}(a) - \sigma) \cdot \left( \frac{\sigma}{1 + |a|} \right)^r, \quad \xi_t^{-1} = \ln(1 + |a|). \quad (11)$$

The correlation length $\xi_t$ is the same as in [6], only with a different prefactor.

**Haldane-antiferromagnet-C.** – Replacing in (10) the spin states $|1\rangle$ by $|2\rangle$ and $|T\rangle$ by $|2\rangle$ we obtain a third matrix product ground state, which is the unique ground state in a 16-parameter subspace of the most general 20-parameter model. The expectation values of $\hat{S}_i^z$-operators are the same as the ones above, except for a factor coming from the higher $\hat{S}_i^z$-eigenstates ($|\pm 2\rangle$ instead of $|\pm 1\rangle$). For other operators, e.g. $\hat{S}_i^x = \frac{1}{2}(\hat{S}_i^+ + \hat{S}_i^-)$, the method of transfer matrices shows that elements like $\langle m_{\mu,\nu}\hat{S}_i^+|m_{\mu,\nu}\rangle$ become relevant. Because the matrix contains elements proportional to $|2\rangle$, $|0\rangle$ and $|2\rangle$ only, this always leads to zero and therefore $\langle \hat{S}_i^x \hat{S}_j^x \rangle \equiv 0$. However, the expectation values of biquadratic operators of this type do not necessarily vanish, e.g.

$$\langle (\hat{S}_i^x \hat{S}_j^x)^2 \rangle = \left( \frac{3 + |a|}{1 + |a|} \right)^2 + 3(\text{sign}(a) + \sigma)|a| \left( \frac{\sigma}{1 + |a|} \right)^r. \quad (12)$$

**Weak antiferromagnet.** – In the following we will show that also other antiferromagnetic phases can be realized by the matrix product technique, e.g. a phase characterized by a vanishing total magnetisation of two neighbouring sites $\langle S_j^z + S_{j+1}^z \rangle = 0$, but with finite single-site magnetisation $\langle S_j^z \rangle \neq 0$. If the sublattice is not fully polarized, i.e. $|\langle S_j^z \rangle| < 2$, the corresponding state will be denoted as weak antiferromagnet.

In order to realize a weak antiferromagnet using the MPA, we introduce the two matrices

$$m = \begin{pmatrix} |1\rangle & x \cdot \sqrt{a} |2\rangle \\ \sqrt{a} |0\rangle & |1\rangle \end{pmatrix}, \quad g = \begin{pmatrix} |T\rangle & \sqrt{a} |0\rangle \\ x \cdot \sqrt{a} |2\rangle & |T\rangle \end{pmatrix}. \quad (13)$$

Using these matrices, two different MPGs can be constructed by assigning the matrices $g$ and $m$ to different sublattices: $|\Psi_0^{(1)}\rangle = \text{tr}(\Pi_{\frac{L}{2}}^t m_{2i-1} \cdot g_{2i})$ and $|\Psi_0^{(2)}\rangle = \text{tr}(\Pi_{\frac{L}{2}}^t g_{2i-1} \cdot m_{2i})$. In the first case to every even lattice site a matrix $m$ is attached and a matrix $g$ to the even numbered sites. In the second case the situation is reversed. Therefore, the ground state is twofold degenerate and each ground state depends on the parameter $a$. The single-site magnetisation alternates from lattice site to lattice site and can be written as

$$\langle S_{m}^z \rangle = -\langle S_{g}^z \rangle = 1 + \frac{|a|(a^2 - 1)}{4 + a^2(x^2 - 1)^2}. \quad (14)$$

For $|x| = 1$ the sub-lattice magnetisation becomes $\langle S_{m}^z \rangle = -\langle S_{g}^z \rangle = 1$. In the limit $|x \cdot a| \rightarrow \infty$ the magnetisation is $\langle S_{m}^z \rangle = 0$ for values $|x| < 1$ and $\langle S_{m}^z \rangle = 2$ for $|x| > 1$. For $|x\sqrt{a}| \rightarrow \infty$
but $|a| \to 0$ a strict Néel order with $|\Psi_0^{(1)}\rangle = |\bar{2}\bar{2} \ldots \bar{2}\rangle$ and $|\Psi_0^{(2)}\rangle = |\bar{2}\bar{2} \ldots \bar{2}\rangle$ is realized. The magnetisations in the $x$- and $y$-direction vanish for the whole subspace,

$$\langle S_x^0 \rangle = \langle S_y^0 \rangle = \langle S_x^2 \rangle = \langle S_y^2 \rangle = 0. \quad (15)$$

The fluctuation $\Delta S^z$ varies in the range from 0 to 1. It takes its maximum for $|x| = 1$ and $|a| \to \infty$. The longitudinal correlation function is given by

$$\langle S_z^1 S_z^r \rangle = (-1)^{r+1} \left( \langle S_z^1 \rangle^2 + A_1 e^{-r/\xi_l} \right) \quad (r \geq 2) \quad (16)$$

and alternates in $r$. It decays exponentially to a constant contribution $\langle S_z^1 \rangle^2$ which is a result of translation invariance breaking. The amplitude $A_1$ is positive and depends on the parameters $a$ and $x$ [16].

The transversal correlation function decays exponentially to zero. Again, the correlation lengths stay finite for all values. In the limits $a \to 0^+$ and $a \to 0^-$ both correlation lengths, the transversal and the longitudinal, diverge. For $a = 0$ the ground-state degeneracy grows exponentially with the chain length.

**Weak ferromagnet.** – The next two matrix product ground states look quite similar to the ones above. The main difference is that the translational invariance is not broken here. With the matrices

$$m = \begin{pmatrix} |1\rangle & \sqrt{a}|2\rangle \\ \sqrt{a}|0\rangle & \sigma|1\rangle \end{pmatrix}, \quad g = \begin{pmatrix} |1\rangle & \sqrt{a}|0\rangle \\ \sqrt{a}|2\rangle & \sigma|1\rangle \end{pmatrix}, \quad (17)$$

the two MPG $|\Psi_0^{(m)}\rangle = \text{tr} \left( \prod_i^L m_i \right)$ and $|\Psi_0^{(g)}\rangle = \text{tr} \left( \prod_i^L g_i \right)$ can be constructed. Due to the spin flip symmetry 2) one has to ensure that both states are ground states of $H$ which then is twofold degenerate. Just as expected, the single-site magnetisation in the $z$-direction reads $\langle \hat{S}_z^1 \rangle = -\langle \hat{S}_z^1 \rangle = 1$ and in the $x$-, respectively $y$-direction $\langle \hat{S}_x^1 \rangle = \langle \hat{S}_y^1 \rangle = 0$. The square of the fluctuation $\Delta \hat{S}_z$ shows the same $a$-dependence as the one from the spin-1 MPG,

$$\left( \Delta \hat{S}_z \right)^2 = \frac{|a|}{1 + |a|} \quad (r \geq 2). \quad (18)$$

The correlation lengths are the same as in the spin-1 case,

$$\xi^{-1}_l = \ln \left| \frac{1 + |a|}{1 - |a|} \right|, \quad \xi^{-1}_t = \ln \left( 1 + |a| \right). \quad (19)$$

Differences can be found in the longitudinal correlation function itself. The possibility to choose either $|\Psi_0^{(m)}\rangle$ or $|\Psi_0^{(g)}\rangle$ leads to a finite contribution to the correlation function

$$\langle \hat{S}_z^1 \hat{S}_z^r \rangle = 1 - \frac{a^2}{(1 - |a|)^2} \left( \frac{1 - |a|}{1 + |a|} \right)^r. \quad (20)$$

This partially polarized state is structurally similar to an antiferromagnetic state. It can be viewed as a Haldane-type state, but with finite magnetization. This is also reflected in the behaviour of the correlation function (20) which agrees with that of the Haldane-AF-B up to the long-range–order part which is zero in the latter case.
Conclusion. – The results presented here show that for a spin-2 chain the spectrum of possible MPG is much larger than for a spin-1 chain. We found three antiferromagnetic phases with unique ground state, exponentially decaying correlation functions and finite excitation gap. Therefore the corresponding phases can be classified as Haldane phases or spin liquids. Their structure is similar to that found in the case of the spin-1 chain [6]. Similar antiferromagnetic phases cannot be constructed for the spin-$\frac{3}{2}$ chain [8]. However, in this case a weak antiferromagnetic and a weak ferromagnetic phase exist. Related states can also be constructed in the present spin-2 case. The weak antiferromagnet shows exponentially decaying correlation functions with long-range order. The ground state is twofold degenerate, reflecting the breaking of translation invariance and leading to a finite sublattice magnetisation. The weak ferromagnet has a twofold degenerate ground state, but full translation invariance. The magnetisation per site in the $z$-direction takes the constant value 1, which is just half of the fully polarised ferromagnet. Interestingly, despite the finite magnetisation, this state is structurally similar to an antiferromagnetic state.

We believe that the exact results presented here are generic for spin-2 chains in a similar way as previous results [6,17] are for spin-1 chains. Here for the isotropic case, i.e. the bilinear-biquadratic chain, an exact solution using OGS is only possible for one point, the AKLT-chain [17]. However, a whole extended phase exists with the same properties. In this sense the exact results allow to study the generic properties of such phases without having to rely on approximate or numerical methods.

Finally we would like to point out that the results found here can be extended to even larger spins just as the Haldane-antiferromagnets-B and -C can be viewed as analogues of the spin-1 states.

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