Dimerization in the anisotropic bilinear-biquadratic Heisenberg model

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Abstract. Two recent publications report different boundaries for the dimerized phase of the bilinear-biquadratic spin-1 Heisenberg model with quadratic Zeeman anisotropy (see Refs. \cite{9} and \cite{10}). We numerically address these discrepancies for the purely biquadratic model with quadratic Zeeman term using methods based on matrix product states (MPS). We extrapolate the results beyond the purely biquadratic model in order to determine the phase boundaries of the dimerized phase and propose a modified phase diagram. Our MPS implementation incorporates SU(2) symmetry explicitly and we discuss its implementation into the MPS representation in the presence of the Zeeman anisotropy.

1. Introduction

The anisotropic Heisenberg model is an immensely useful model for the study of many body (spin) systems. For a one-dimensional lattice with \( N \) sites it is given by

\[
h_{i,i+1} = \cos \theta \vec{S}_i \otimes \vec{S}_{i+1} + \sin \theta (\vec{S}_i \otimes \vec{S}_{i+1})^2 + D (S^z_i)^2
\]

and includes an exchange interaction between sites \( i \) and \( i+1 \) controlled by the parameter \( \theta \) as well as Zeeman anisotropy with strength \( D \). The \( S^\nu_i \) are spin-\( s \) SU(2) matrix representations with \( \nu = x, y, z \), and \( i = 1, \ldots, N \) and \( N + 1 \rightarrow 1 \) for periodic boundary conditions.

This model has been studied extensively using field theoretical and numerical methods as a function of the parameters \( \theta \) and \( D \), and it can be experimentally realized in various crystalline materials as well as using trapped ultracold gases. In particular, the model was instrumental to establish the importance of topological terms in low energy field theories: For the antiferromagnetic bilinear model (\( \theta = 0 \)) Haldane \cite{1, 2} found a surprising difference between integer and half-integer spin chains, which was later related to a topological \( \theta \)-term in the low energy field theory. More recently, a topological analysis \cite{3, 4, 5} was undertaken for the dimerized region \((-3\pi/4 < \theta < -\pi/4)\), which for a long time created quite some confusion with regard to a possible nematic phase as conjectured by Chubukov \cite{6} for \( \theta \) close to the transition point at \( \theta = -3\pi/4 \).

In order to establish and clarify such rather non-trivial features of the model, numerical investigations are absolutely essential: Most prominently, the development of the DMRG method \cite{7} in the early nineties proved very useful in order to support the results obtained using field theoretical methods, e.g. the celebrated Haldane gap in spin-1 chains \cite{8}. In this respect,
it is rather interesting to note that the extension of the dimerized phase in the \((\theta, D)\)-plane is still rather controversial. In fact, two recent numerical investigations \([9, 10]\) find very different extensions of the dimerized phase as a function of \(\theta\) and the Zeeman strength \(D\). We addressed these discrepancies in a recent work \([11]\) using a matrix product state (MPS) algorithm for periodic boundary conditions with consideration of SU(2) symmetry \([12, 13, 14]\). In particular, we made extensive calculations at \(\theta = -\pi/2\) and developed from these results a modified phase diagram for the dimerized region. In the present note we will extend these investigations and discuss the resulting phase diagram and, furthermore, comment on the numerical method and its numerical complexity.

At \(\theta = -\pi/2\) and \(D = 0\) only the biquadratic term remains in (1) which is SU(3) symmetric \([15, 16]\), i.e. it may be rewritten as a bilinear model in terms of the three-dimensional Gell-Mann SU(3) ‘quark’ (\(\lambda\)) and ‘antiquark’ (\(\bar{\lambda}\)) triplet representations,

\[
h_{i,i+1} = -8\lambda_i \otimes \bar{\lambda}_{i+1} - \frac{4}{3} \mathbb{1}.
\]  

The quadratic Zeeman term, which in terms of Gell-Mann matrices is given by \(2D(1/3 \mathbb{1} + \lambda_3 - \lambda_8)\), reduces the symmetry from SU(3) to SU(2), i.e. the Gell-Mann triplet splits into an SU(2) spin-\(\frac{1}{2}\) duplet and one singlet at each site. We shall call this SU(2) subgroup \(v\)-spin. This SU(2) symmetry holds only at \(\theta = -\pi/2, \pi/2, -3\pi/4, \text{and } \pi/4\), and is different from the \(D = 0\) SU(2) symmetry of the Hamiltonian (1), which we shall call \(s\)-spin. The latter reduces to U(1) at all \(\theta\) due to the Zeeman term. Since a continuous symmetry cannot be broken in one dimension \([17, 18]\), we developed a matrix-product algorithm which incorporates \(v\)-spin symmetry explicitly in the ansatz for the MPS similar to our treatment of SU(2) symmetric MPS presented in Ref. \([14]\). Details will be discussed in section 2.

By now it is accepted \([5]\) that the isotropic \((D = 0)\) bilinear-biquadratic spin-1 system is dimerized for all \(\theta\) between the two critical points \(\theta = -3\pi/4\) and \(\theta = -\pi/2\). Using the results at \(\theta = -\pi/2\) as a guide, we develop and discuss in section 3 a modified phase diagram for the anisotropic model in the dimerized region.

2. SU(2) symmetric algorithm for \(v\)-spin
As was mentioned above, at \(\theta = -\pi/2\) the anisotropic bilinear-biquadratic Heisenberg model is SU(2) symmetric. This is not immediately obvious from the standard spin representation given in Eq. (1), but can be understood from the SU(3) representation given in Eq. (2), which contains \(v\)-spin as a subgroup. The Zeeman term reduces the SU(3) symmetry to this SU(2) subgroup and, as a consequence, the SU(3) multiplets split into SU(2) multiplets, e.g. an SU(3) triplet splits into a SU(2) doublet and a singlet, and an SU(3) octet splits into 2 singlets, two doublets and one triplet. Therefore, the obtained states may be labeled by SU(2) \(v\)-spin quantum numbers. The U(1) subgroups of \(v\)-spin and \(s\)-spin are related by \(S_z = 2v_z\). This splitting of the SU(3) multiplets can be seen in calculated spectra as exemplified in Fig. 1.

In another recent paper \([14]\) we described in detail an algorithm for SU(2) symmetric matrix product states (MPS) with periodic boundary conditions. It is constructed from tensors separated into structural and degeneracy parts, \(C\) and \(M\), respectively,

\[
M_{(jt)_{m},(jt')_{m'}}^{(j't'm')_{m}} = M_{(jt),(jt')}^{(j't'm')} C_{m,m_s,m_t}^{j,s,j',t}.
\]  

In order to form the MPS, \(N\) such tensors are contracted over the virtual spin indices \((jtm)\) and \((j't'm')\). The (variational) parameters of the MPS are the matrix elements of the degeneracy tensors \(M\), while the structural part is given by a Clebsch-Gordan coefficient as detailed in Ref. \([14]\). Analogous expressions are defined for matrix product operators (MPO). The goal of the MPS algorithm we developed is the explicit elimination of all structural tensors. This is
The essential structure of the spectrum remains very similar for larger systems due to structural part $C$ for each possible combination of quantum numbers $j, j'$ forms a SU(2) spin-1 matrix representation. However, for $v$-spin we do not place a spin-1 representation at each site but the direct sum of a spin-1/2 and a spin-0 representation. This follows from the fact that $v$-spin is a subgroup of SU(3) with a Gell-Mann triplet as basic representation. This fact has a number of consequences for the MPS algorithm, and a slight modification to the algorithm described in Ref. [14] is required. These changes are rather technical and we do not describe the details here.

We just want to mention some essential points: while the general structure of the MPS given in Eq. (3) can be maintained, it is necessary to introduce additional loops over $s$ with $s = 1/2$ and $s = 0$. Secondly, one has to slightly modify the definition of the representation for the matrix product operator MPO (see Eq. (19) in Ref. [14]) again in order to take care that it now has off-diagonal elements in $s$ and $s'$. Finally, one has to develop the explicit reduced representation of the MPO for the bilinear-biquadratic Heisenberg model including the Zeeman term $D$ which would replace the explicit representations given in Appendix A of Ref. [14]. With these considerations in mind, it is not difficult to fill in all technical details and construct the reduced MPO representation and the corresponding algorithm.

Finally, a few remarks about the efficiency of the calculations: The complexity of the calculations is essentially determined by the choice of the quantum numbers (virtual indices) $(jt), (jt')$ with $j, j' \in \{0, 1/2, 1, 3/2, 2, \ldots\}$ and $t \in \mathbb{N}$. Here, $t$ and $t'$ are the degeneracies of $j$ and $j'$ we choose for our MPS representation. A priori these degeneracies are not restricted, and there is no upper limit for $j$ or $j'$, respectively. They have to be chosen as small as possible but such that the algorithm converges, and this choice is partly a matter of trial and error. A particular choice we call a degeneracy set $T = \{t_0, t_1, \ldots, t_{2j_{\text{max}}}\}$, and for the calculations of the spectra shown in Fig. 1 they are listed in the table shown to the right of the figure.

Spectra for systems with more than $N = 30$ spins look rather similar as in Fig. 1, of course.
the gaps get smaller, and with increasing system size the lowest gap(s) may close. In fact, for dimerization to happen, the lowest states must be degenerate singlets. And as we have shown in detail in our previous publication we find degenerate singlets or degenerate singlets together with a triplet for $D < 0.25$. For $D > 0.25$ the gap does not close, and the system is not dimerized.

3. Boundaries of the dimerized phase of the Heisenberg model with Zeeman anisotropy

The boundaries of the dimerized phase have been studied by Rodriguez et al. [9] using level spectroscopy and by De Chiara et al. [10] from a direct calculation of the dimerization order parameter. The results are not in agreement. In our recent paper [11] we addressed these discrepancies and pointed out the basic reason why level spectroscopic results from finite system calculations as presented in Ref. [9] are problematic: Dimerization only occurs if the lowest two singlets are degenerate in the thermodynamic limit. However, we find that the gap between the lowest two singlets does not close for all $D$ larger than some small value close to zero. More details may be found in Ref. [11].

Here we concentrate on calculations of the dimerization order parameter \( \tilde{D} = \frac{1}{N} \sum_i (-1)^i h_{i,i+1} \). Results for the dimerization correlator are presented in Fig. 2 (left). For $D = 0$ the dimerization is well-known from the literature [19, 20], $D_\infty = \frac{\sqrt{2}}{2} \prod_{\alpha=1}^{\infty} \tanh^2 (n \arccosh^2 3) \simeq 0.562$. Our results for 30, 40 and 50 sites at $D = 0$ can be fitted very well by the function [21, 22]

\[
D(N) = D_\infty + c N^{-\alpha} \exp(-N/2\xi) \]

with $\alpha = 1$. From the fit we obtain $D_\infty \simeq 0.568$ in good agreement with the Bethe Ansatz, and a large correlation length $\xi \simeq 20.2$. A very similar result for the correlation length was obtained in Ref. [21] from the lowest energy gap.

The dimerization correlator is determined from the two lowest $v = 0$ eigenstates with different momenta for 30, 40, and 50 sites. The red line in Fig. 2 (left) shows the extrapolation to the thermodynamic limit. The black cross indicates the Bethe ansatz value at $D = 0$ and $N \to \infty$. The dimerization is strictly zero for $D \gtrsim 0.03$. The green line shows the result obtained by De Chiara et al. [10] at $\theta = -0.6\pi$ (the dashed part is extrapolated from their data). Our results confirm the prediction of De Chiara et al. that the dimerization persists up to large negative values of $D$.

Let us now transfer these results at $\theta = -\pi/2$ into the phase diagram shown in Fig. 2 (right) and combine them with insights we obtained from the spectral analysis of Ref. [11]. We find...
that a gapped dimerized phase exists in the parameter range $D^- < D < D^0$ with $D^- \approx -0.30$ and $D^0 \approx 0.025$. Moreover, we identify a gapless dimerized phase which extends from $D^-$ to large negative $D$. While this confirms the results of De Chiara et al. [10], who predicted a small dimerization even below $D < -2.0$, the existence of both a gapped and a gapless dimerized phase is reported here for the first time. The transition between these two dimerized regions occurs at $D^-$ which was erroneously identified as the boundary of the dimerized phase in Ref. [9]. At the upper end of the dimerized region close to $D^0$, the dimerization sharply drops to zero and a gap opens between the two lowest singlet states marking the transition to a non-dimerized phase. We do not see a phase transition at $D^+$ which was identified as the upper dimerized phase boundary in Ref. [9]. These findings for $\theta = -\frac{\pi}{2}$ are graphically represented on the vertical axis of the phase diagram shown in Fig. 2 (right), where the various transition points are marked by black dots.

We now qualitatively extrapolate these results for $\theta$ in the parameter interval $I = [\frac{\alpha}{2}, -\frac{\alpha}{2}]$, separately for positive $D$ and negative $D$, guided by general considerations and the calculations presented in Refs. [9] and [10]: By now it is rather well established that for $D = 0$ the bilinear-biquadratic spin-1 model has a dimerized ground state in the whole parameter interval $I$. In particular, a nematic non-dimerized phase close to the ferromagnetic transition has been ruled out [4, 5]. At large negative or positive $D$ the system is not dimerized. This follows from simple analytical arguments [10].

At large positive $D \gg 1$ the system is in the gapped large-$D$ phase [10], and the transition between the dimerized phase to a non-dimerized phase happens at small positive $D$ for all $\theta \in I$ [10]. This we confirmed in the present paper for $\theta = -\frac{\pi}{2}$. Furthermore, we recently made a number of calculations at various $\theta$, which clearly show that the transition to the dimerized phase is at $D < 0.02$. In fact, one expects that the system is in an Ising nematic phase for all $D > D^0$ as indicated by the white region above the blue shaded region in Fig. 2 (right) as there are no gaps closing in the spectrum. However, it is expected from the results of Ref. [9] that the leading excitation changes from $S_z = 0$ for $D < D^+$ to $S_z = \pm 1$ at $D > D^+$ as indicated by the blue dashed lines in the phase diagram. According to Ref. [5] the dimerization is related to the density of disclinations created in the spin system. Consequently, such topological defects should be absent for $D > D^0$.

For large negative $D$ the system is in a gapless critical (XY nematic) phase for $-\frac{3\pi}{4} < \theta < -\frac{\pi}{4}$ and in a gapped Neel phase for $-\frac{\pi}{2} < \theta < -\frac{\pi}{4}$ [10]. For small and intermediate negative $D$, the XY nematic and the Neel phases are separated by dimerized phases as indicated by the blue, red, and green shaded regions in Fig. 2 (right). It is expected that the gap between the lowest two singlets closes in all theses colored regions making them dimerized. In addition, in the red region also the gap to the next triplet closes, i.e. one expects a 5-fold degenerate ground state and vanishing staggered magnetization. This corresponds to our findings at $\theta = -\frac{\pi}{2}$. In the dimerized green shaded region, we expect an open gap to the triplet state and a non-zero staggered magnetization. The line between the red and green dimerized sectors separates magnetically staggered and non-staggered phases. This must be confirmed in detail by further calculations.

4. Conclusions
In this paper we elaborated on our proposal [11] for a modified phase diagram in the dimerized region of the bilinear-biquadratic spin-1 Heisenberg model and resolved discrepancies for the phase boundaries reported in previous work [9, 10]. The modified phase diagram is presented in our Fig. 2, which indicates that for positive anisotropy parameter $D$ the system is not dimerized except at very small positive $D$. Our proposal is based on numerical results from matrix product state calculations, which explicitly maintain SU(2) symmetry.
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