Absence of string order in the anisotropic $S = 2$ Heisenberg antiferromagnet

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In this paper we study an antiferromagnetic Heisenberg $S = 2$ quantum spin chain at $T = 0$ with both interaction and on-site anisotropy,

$$H = \sum_i \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + J_z S_i^z S_{i+1}^z + D(S_i^z)^2.$$

While the phase diagram of this chain for $S = 1$ and the isotropic point for $S = 2$ are by now excellently understood, contradictory scenarios exist for the $S = 2$ anisotropic phase diagram, which imply completely different mechanisms of the emergence of the classical $S \to \infty$ limit, hence the importance of the question. One main scenario predicts the emergence of a cascade of phase transitions not seen in the $S = 1$ case, based on an analysis using the Affleck-Kennedy-Lieb-Tasaki model. Another scenario is in favor of an almost classical phase diagram for $S = 2$, from which the $S = \infty$ phase diagram evolves quite trivially; the $S = 1$ case then emerges as very special with its dominant quantum effects. Numerical studies have so far not been conclusive.

Using the Density Matrix Renormalization Group, we study gaps and correlation functions in the anisotropic $S = 2$ chain. The question of the existence of hidden topological order in the anisotropic $S = 2$ chain is emphasised, as it distinguishes between the proposed scenarios. Careful extrapolation allows us to show that the topological order is zero in the thermodynamical limit in all disordered phases, in particular in the new phase interposed between the Haldane and large-$D$ phases. The decay of the hidden order is substantially faster than that of $S^+ S^-$ correlations and excellently fitted by power-laws typical of massless phases. This excludes the AKLT-model based scenario in favor of an almost classical phase diagram for the $S = 2$ and thus higher spin chains.

I. INTRODUCTION

Interest in quantum spin chains as examples of low-dimensional strongly correlated quantum systems was greatly revived in 1983 by Haldane’s famous conjecture of a fundamental difference between half-integer and integer quantum spin chains, a phenomenon without equivalent in higher dimensional systems.

In the meantime, Haldane’s conjecture has been firmly established, while not rigorously proven. The numerical values of the predicted gaps and finite correlation lengths for isotropic integer spin chains are by now extremely well known both in the $S = 1$ case and the $S = 2$ case, which constitute the extreme quantum limit. Furthermore, for both cases Haldane’s predictions of a massless relativistic dispersion relation have been confirmed.

Haldane’s conjecture was derived from a non-linear quantum sigma model, which is an effective low-energy continuum theory of the isotropic Heisenberg model in the semiclassical limit $S \to \infty$. It does not provide immediate insight in the ground state of integer spin chains.

The Affleck-Kennedy-Lieb-Tasaki (AKLT) model provides a profound physical understanding of gapped spin liquids. The AKLT model is the Hamiltonian which gives rise to the following exact ground state: each spin of length $S$ is decomposed into $2S$ completely symmetrized $S = \frac{1}{2}$ spins. Pairs of such spins on neighboring sites are linked up by singlet bonds, giving rise to $S$ singlet bonds between sites. In the case of $S = 1$, all important features of the isotropic Heisenberg model and the AKLT model, which has the Hamiltonian

$$H_{\text{AKLT}}^{S=1} = \sum_i S_i S_{i+1} + \frac{1}{3} (S_i S_{i+1})^2 \quad (1)$$

are in qualitative agreement.

A particularly striking feature of both models is the existence of a hidden non-local topological order, also known as string order, which does not vanish in the limit $|i - j| \to \infty$. For the AKLT model, the value is $\frac{1}{9}$, for the Heisenberg model $0.37432\ldots$. In the case of a $S = 1$ chain, it describes a hidden antiferromagnetic order of $S^z_i = \pm 1$ spin states, which is diluted by arbitrary numbers of interposed $S^z_i = 0$ spin states and thus not seen in the antiferromagnetic order parameter.

The existence of the hidden order can further be associated with the breaking of a $Z_2 \times Z_2$ symmetry in the Haldane phase, as well as with the existence of a fourfold degenerate ground state of an open Heisenberg chain in the Haldane phase. For $S = 1$, the success of the AKLT-model can be understood as it is a quantum disordered point, a remnant of a classical phase transition. For higher spins, as we will see, both the existence of hidden order and its signification are not clear.

In this paper, we want to make progress towards understanding how the classical phase diagram emerges out of the substantially different $S = 1$ phase diagram. Examining different scenarios, we will see that their fundamental difference regards whether or not there exists hidden order in the $S = 2$ phase diagram for suitable
anisotropies. Our results will allow to decide quite clearly in terms of a scenario without hidden order for \( S = 2 \). We finish by addressing briefly why the AKLT model is not successful in explaining the anisotropic \( S = 2 \) phase diagram.

II. \( S = 1 \) AND \( S = \infty \) PHASE DIAGRAMS

In real physical systems, such as NENP as the quintessential \( S = 1 \) spin chain, anisotropies are always present, in the case of NENP an easy-plane on-site anisotropy \( D \approx 0.18 \). In order to link experiments to theory, it is therefore necessary to understand the phase diagram with anisotropies. At the same time, this may provide deeper theoretical insight into the interplay of the different phases. \( S = 1 \) phase diagram. The \( S = 1 \) phase diagram, as the physically most relevant one with at the same time the strongest quantum effects for an integer spin chain, has been studied extensively and is by now extremely well understood. Let us summarize the main features (Figure 1).

Both for substantially strong \( J^z \) anisotropy and sufficiently small \( D \), one finds Ising-like ordered (anti)ferromagnetic phases, depending on the sign of \( J^z \). The transition lines are not very far from those in the classical limit (see below).

All other phases are disordered, but otherwise physically quite distinct: For large \( D \), all \( S^z \neq 0 \) states are suppressed and a singlet phase emerges, with a gap proportional to \( D \), as the gap is essentially the energy to excite one spin to \( S^z = \pm 1 \). Below that, there are two phases. Their separation line is strictly \( J^z = 0 \), as first shown by den Nijs and Rommelse, and later on confirmed numerically with increasing precision. For \( J^z > 0 \), there is a gapped quantum liquid, the Haldane phase, including the isotropic Heisenberg model, with the properties described above. For \( J^z < 0 \), there is an XY-phase with power-law decay in the \( \langle S^+_i S^-_j \rangle \) correlations. In fact, the XY phase decomposes into two phases with different correlation functions, linked by an Ising-like transition. Phase transitions out of FM order are first order, from AFM order to the large-\( D \) phase first order, from Haldane to XY, and from XY to large-\( D \) Kosterlitz-Thouless like, and the Haldane to large-\( D \) transition has been likened to a preroughening transition in RSOS models.

- \( J^z > 0 \) and \( D < J^z - 1 \): ordered antiferromagnetic Ising-phase (AFM)
- \( J^z < 0 \) and \( D < -J^z - 1 \): ordered ferromagnetic Ising-phase (FM)
- \( D > |J^z| - 1 \): ordered antiferromagnetic XY phase (XY): all spins in-plane

III. EMERGENCE OF THE CLASSICAL LIMIT

How does this classical phase diagram emerge from the \( S = 1 \) phase diagram? In recent years, various scenarios have been proposed.

FIG. 1. \( T = 0 \) phase diagram of the \( S = 1 \) anisotropic Heisenberg antiferromagnet. Transition lines are schematic; the XY-Haldane transition line is at \( J^z = 0 \) exactly; the FM-XY transition line includes \( D = 0 \), \( J^z = -1 \). For \( J^z = 1 \), the Haldane-large-\( D \) transition is at \( D = 0.99(1) \); for \( D = 0 \), the Haldane-AFM transition at \( J^z \approx 1.2 \). The XY phase actually comprises two different XY phases 1 and 2.

FIG. 2. \( T = 0 \) phase diagram of the classical anisotropic Heisenberg antiferromagnet. All transition lines are exact.
FIG. 3. Phase diagram for $S > 1$ as predicted by bosonization. The figure is not to scale. Adapted from Ref. 20.

1. Bosonisation predicts for all integer spins $S$ essentially the same scenario as for $S = 1$ (Figure 3). Bosonisation can be expected to predict the nature of the phases found and their topology (i.e. which phases are joined by a transition), but not to yield quantitative values for the phase boundaries.

For $S = 1$, bosonisation indeed predicts all phases and the correct topology of the phase diagram; it merely misses that the large-$D$, AFM and FM phases meet respectively for very large anisotropies, beyond the limit of applicability of bosonisation. For higher spins, it is predicted in particular that for an isotropic exchange interaction $J^z = 1$ there is exactly one transition from the Haldane phase to the large-$D$ phase for $D \rightarrow \infty$. From other arguments it can be concluded that for large $S$ the large-$D$ phase will pushed out to $D \rightarrow \infty$, whereas the gap of the Haldane phase vanishes; in the $S \rightarrow \infty$ limit the gapless XY-phase emerges (but for the isotropic point, any $D > 0$ will then favour in-plane spins for $J^z = 1$).

Numerical studies are by now in excellent agreement that already for the $S = 2$ case there are not only two, but three phases when taking $D \rightarrow \infty$ for positive $D$ and $J^z = 1$. While the results of Ref. 23 are not reconcilable with bosonisation, those of Refs. 7 and 30 could be interpreted as being in accordance with bosonization, if one allows for a major deformation of the bosonization phase diagram. In the scenario we are going to show numerically below, bosonisation will be found to predict the correct phases, but we will also see that the necessary deformation of the bosonization phase diagram changes it almost beyond recognition.

2. A second scenario was proposed by Oshikawa in the spirit of the Affleck-Kennedy-Lieb-Tasaki (AKLT) model (Figure 4).

Oshikawa has shown that the hidden topological order parameter (the string order parameter) disappears exactly in the AKLT model, describing the isotropic chain, for all even integer spins $S = 2, 4, \ldots$, while it yields a finite value for odd integer spins $S = 1, 3, \ldots$. On the other hand, Oshikawa argues that the effect (assuming for the moment an isotropic exchange interaction, $J^z = 1$) of an increase in the easy plane anisotropy $D > 0$ is to successively suppress the large $S^z$ states: first $\pm S$, then $\pm (S - 1)$, and so on. This yields in his analysis a succession of spin chains with effective spin lengths $S, S - 1, \ldots, 1, 0$. The envisaged succession of spin models can be schematically drawn in the AKLT picture as in Figure 4.

As the string order parameter should be alternatingly zero and non-zero in the even and odd integer spin chains, Oshikawa predicts a succession of $S + 1$ phases with $S$ phase transitions, beginning with the isotropic Haldane phase (spin length $S$) and ending with the large-$D$ phase, assimilated to a spin length 0. The transitions are characterized by the (dis)appearance of a finite string order parameter. The classical limit would then emerge by a softening of the quantum phase transitions and a disappearance of possible gaps in the $S + 1$ phases.

The AKLT scenario works excellently for the $S = 1$ case; and it is extremely well established that a similar scenario, also proposed by Oshikawa, of multiple phase transitions works extremely well to describe successive phase transitions in an isotropic Heisenberg integer spin antiferromagnet with increasingly strong dimerization of the interaction bonds, in excellent agreement with field theoretical predictions and numerical verification. All this makes this a very strong scenario.

The existence of an intermediate phase, as should exist for $S = 2$, was first established in Ref. 23 and later confirmed in Refs. 24 and 30. Oshikawa et al. using Quantum Monte Carlo on systems up to $L = 160$, claim to see, at least for $D \approx 1.2$ and $J^z = 1$, a non-vanishing string order parameter, which they extrapolate to a thermodynamic limit of $1 \times 10^{-3}$ at that particular point. They interpret furthermore the behavior of spin-spin correlations as indicative of a phase transition for $J^z \approx 0$. Furthermore, a sign-alternation exists in the string order at the isotropic point, but not at $D = 1.2$. These results would support Oshikawa’s scenario of multiple transitions.
3. A third scenario results from numerical work by Schollwöck et al. (Figure 6). It actually has a precursor in the works of Khveshchenko and Chubukov. They argue that the large-$D$ phase moves as $S^2$ up to $D \to \infty$ for $S \to \infty$, while the Haldane phase recedes from the isotropic point. The XY phase already present in the $S = 1$ phase diagram vanishes in the part of the phase diagram; in the XY phase the hidden order parameter is zero in the thermodynamic limit. The $S = 1$ case with its strict $J^z = 0$ transition line between XY and Haldane phase emerges thus as particular. Numerically it is found that the Haldane phase is reduced to a small stripe next to the antiferromagnetic phase and squeezed out for $S \to \infty$, as the gap is suppressed exponentially as $e^{-\pi S}$; the large-$D$ phase moves up to $D \to \infty$, and the classical phase diagram emerges in a particularly simple fashion. There is no clear information on the behavior of the Haldane phase at its two end points. It is not clear whether (i) the Haldane phase touches the large-$D$ phase at its two end points and (ii) whether XY and AFM phase meet at its left end. If both are true, then not only the same phases, but also the same phase boundaries as in the bosonization picture emerge; the phase diagram looks still quite different.

Numerically, the existence of an additional phase between the Haldane and the large-$D$ phase has been demonstrated using the DMRG. For $J^z = 1$, the transition points were placed at $D_{c_1} = 0.04(1)$ and $D_{c_2} = 3.0(1)$. The intermediate phase was identified as gapless, with exponentially decaying $\langle S_i^z S_j^z \rangle$ correlations, power-law like decay in the $\langle S_i^x S_j^y \rangle$ correlations, and a vanishing string order parameter, in support of the above picture. However, available computational resources did not allow a very precise determination of the quantities involved (lengths up to 200, keeping 200 block states in the DMRG).

**IV. STRING ORDER IN THE $S = 2$ PHASE DIAGRAM**

1. Before we discuss our results on gaps and correlation functions, a remark on the calculation of the string order parameter is in order, as the crucial information is whether it is finite or not in the thermodynamic limit. Conventionally, the string order parameter is defined by
\[ O(i, j) = \langle S_i^z e^{i\pi \sum_{k=i}^j S_k^z} S_j^z \rangle. \]  
\[ O^2(i, j) = \langle S_i^z e^{i\pi \sum_{k=i}^{j-1} S_k^z} S_j^z \rangle, \]  
\[ O^0(i, j) = \langle S_i^z e^{i\pi \sum_{k=i}^{j-1} S_k^z} S_j^z \rangle. \]

This means that the exponential string includes one of the two spins correlated. In the \( S = 1 \) literature, numerically often two alternative quantities are calculated: an order parameter with a string including both correlated spins,

\[ \text{and an order parameter including none of the correlated spins,} \]

\[ -O^2(i, j) = O(i, j) = -O^0(i, j) \]  
strictly. In the \( S = 2 \) case, this is no longer true: \( S^z = \pm 2 \) and \( S^z = \pm 1 \) lead to different sign behavior in the three definitions. It is however, if computational resources are stretched to their limit, more efficient for memory consumption reasons to calculate either \( O^0 \) or \( O^2 \) in the DMRG method because then the string can be decomposed into two symmetric parts, if \( i \) and \( j \) are chosen symmetric about the chain center of an open chain. Only one needs to be stored then.

We have checked in lower precision calculations (200 states kept, length 200) that in the region of importance the following inequality is always observed:

\[ |O^2(i, j)| \leq |O(i, j)| \leq |O^0(i, j)|. \]

The very small difference in these correlations decreases with increasing \(|i - j|\) both absolutely and relatively. Therefore, in the following, we always refer to the calculation of \( O^0(i, j) \). It provides both an upper bound to \( O(i, j) \) and converges to the same thermodynamic limit for \( i - j \to \infty \). In fact, on all our plots the difference between the various correlations would be invisible to the eye.

2. An observation that can be made numerically is that the string order parameter at \( D = 0 \), \( J^z = 1 \) decays with alternating sign, whereas in the intermediate phase it decays with no sign-alternation. This might be attributed to a substantial difference between the various \( S = 2 \) phases, as it has been done in Ref. [22]. Alternatively, this might naively be attributed to the fact that \( D > 0 \) suppresses both large \( S^z \) values and leads to a very fast decay of \( S^z S^z \) correlations: With \( J^z = 1 \), spin-spin correlations are antiferromagnetic for arbitrary \( D \). This introduces a fundamental sign-alternation in the string order. What is effectively observed, now depends on the string: For \( D \approx 0 \) and \( J^z = 1 \), the close neighbourhood of the Ising AFM phase indicates that \( S^z = \pm 2 \) states dominate in the string, contributing factors 1. The string order parameter therefore exhibits sign-alternation. When \( D \) is successively increased, \( S^z = \pm 1 \) and then \( S^z = 0 \) states dominate, introducing a sign alternation in the string for the former and no alternation for the latter case, such that the total order parameter is non-alternating and then alternating again.

Calculating chains up to length \( L = 200 \) with the DMRG, we find for \( D \geq 0.02 \) that the string order parameter shows sign-alternation for small distances, but no sign-alternation for longer distances. As we find (see below) a rather strong dependence of the string order parameter on the total system size if the string length becomes of the order of the system size, we have localized this “crossover” of the sign-behavior for various total system lengths. For \( D \geq 0.03 \), the crossover point is sufficiently small compared to the total system length that it may be considered almost converged; the numerical data does not exclude the possibility that the sign crossover can already be observed for smaller \( D < 0.02 \). We find crossover points as in Table [3].

The sign crossover can be attributed to rather strong short ranged Neel like order, which is still present for small \( D \), but does not survive for larger distances. It is of no importance whatsoever for larger values of \( D \). The change in behavior is gradual and not directly linked to the critical value of \( D = 0.043 \) for the large-\( D \) phase, the second change in sign behavior is not observed up to \( D = 3.5 \), which is already deep in the large-\( D \) phase (gap of the order 0.05).

This establishes that there is no direct relationship between the phase transitions and the sign behaviour of the string order; a non-alternating decay is no unique feature of the intermediate phase.

3. Furthermore, we have compared the decay of various correlation functions in the XY phase. In all points, we find a very fast exponential decay of \( S^z S^z \) correlations, and power-law decays in the string order and the \( S^z S^- \) correlations. The decay of the string order is much faster than that of the typical XY phase correlations, even though the difference decreases towards the upper right corner of the XY phase. We see no change in behavior between \( J^z < 0 \) and \( J^z > 0 \). To give an example, decays follow laws \( x^{-\alpha} \), with \( \alpha = 0.13 \) for \( J^z = -0.5 \), \( D = 1.0 \) and \( \alpha = 0.18 \) for \( J^z = 0.5 \), \( D = 1.0 \) for the \( S^z S^- \) correlations and \( \alpha = 2.11 \) for \( J^z = -0.5 \), \( D = 1.0 \) and \( \alpha = 1.47 \) for \( J^z = 0.5 \), \( D = 1.0 \) for the string order. This is indicative of the XY nature of the intermediate phase.

4. Before we discuss results on the string order in the intermediate phase, let us first try to locate it with more precision. We consider only the part of the phase diagram with \( J^z > 0 \) and \( D > 0 \) (Figure [8]).

The transition line from the AFM phase to the Haldane or large-\( D \) phases can be easily located with the behavior of the \( S^z S^z \) correlation function. Considering chains up
to length \( L = 300 \), this transition line was determined with a precision of \( \pm 0.05 \) in the critical \( D \)-value.

The Haldane phase is very narrow (cf. former results for \( J^z = 1.0 \approx 0.5 \)), approximately 0.1 wide in units of \( D \). A more precise determination has not yet been carried out, only at \( J^z = 1.0 \) (considered above) and \( J^z = 3.3 \) (see below).

The crucial question is the location of the transition from the intermediate to the large-\( D \) phase, because the gap in the large-\( D \) phase opens exponentially slow. Here, we have calculated the gap in high-precision calculations (300 states kept, length 300) for various values of \( D \) for \( J^z = 1; 2.5; 3.3 \). The fact that the gap is very small (or vanishes) implies an extremely large or divergent \( \xi \), which has the advantage that a simple \( L^{-1} \)-extrapolation of the gap should provide a rather precise estimate of the gap (cf. the detailed discussion of such extrapolations in Refs. 7, 8). DMRG errors cancel to some extent as both ground and first excited state have similar truncation errors (approximately \( 10^{-8} \) or better for \( L = 600 \) and \( M = 400 \) states kept). Variation of the number \( M \) of kept states reveals that we overestimate gaps slightly. Extrapolation in \( M \) as well as gap calculations for points where the gap is known to disappear let us estimate that gap values \( \Delta > 0.001 \) are really finite. Consider Figure 7. For \( J^z = 3.3 \), the truncation error is comparatively large, \( \approx 2 \times 10^{-8} \). The very small gaps observed leave two scenarios: (i) between the Haldane phase (\( D \approx 2.65 \)) and the large-\( D \) phase (for \( D \) larger than \( D \approx 3.0 \)) there is a small intermediate phase; (ii) Haldane and large-\( D \) phase meet directly, at \( D \approx 2.8 \). For smaller \( J^z \), the two phases can be clearly separated, still there is some uncertainty as regards the transition to the large-\( D \) phase. This leads us to the diagram shown in Figure 8: the upper transition line might in reality be somewhat lower (by no more than 0.2 units in \( D \) close to the upper right end of the XY phase; the transition point for \( J^z = 1 \) is essentially exact). In any case, if we overestimate the size of the intermediate phase, there is no finite string order in the true intermediate phase if we don't find it in our oversized one. So our argument is not weakened. In fact, most of our points are far from the transition line anyways.

5. Within the intermediate phase thus identified we are now going to calculate the thermodynamic limit of the string order for a large number of points.

To discuss the possibility of an Oshikawa-like phase in the upper right corner, we will systematically investigate points for large \( J^z \).

Our procedure to calculate the thermodynamic limit of the string order parameter is as follows. Using the DMRG, we calculate for a given set of \((J^z, D)\) the string order parameter

\[
O(N, L, M) = \langle S_i^z e^{i\pi \sum_{k=+1}^{L-1} S_j^z} \rangle
\]

with \( N = |i - j| \) \( i, j \) symmetric about the center of an open chain of length \( L \) studied using a reduced Hilbert space of \( M \) states per block.

FIG. 7. Location of extrapolated gaps \( \Delta \) for \( J^z = 3.3 \) vs. anisotropy \( D \). For \( D = 2.6 \), the chain is in the AFM phase. The bottom line \( \Delta = 0.001 \) indicates our estimate of the precision limit. For smaller gaps, it cannot be clearly decided whether they are finite. The gapped phase on the left is the Haldane phase, the gapped phase on the right the large-\( D \) phase. Note that the gap curve would be almost flat, if the same scale were used for \( D \) and \( \Delta \).

FIG. 8. Location of points which were calculated for chain lengths \( L = 600 \), keeping 400 states for the DMRG. The transition lines were obtained numerically; the AFM transition line is determined up to \( D = D_c \pm 0.05 \) or better; the Haldane phase has a width of \( \approx 0.05 \) or smaller and is thus hardly distinguishable from the XY phase, also due to the small gap. The \( D \) transition line is possibly slightly too high, as DMRG has difficulty in seeing extremely small gaps.

To obtain the thermodynamic limit \( N \rightarrow \infty \), we first have to eliminate the DMRG typical dependence on \( M \).
of an order parameter for given $N$, $L$. This extrapolation can be done by fitting the string order against the DMRG truncation error. We find that for $M = 400$ the errors in the extrapolated results are of no relevance to the following extrapolations.

\[
O(N) = C(J^z, D)N^{-\alpha(J^z, D)},
\]

as expected in a critical phase, where $\alpha$ varies slowly. The exponent $\alpha$ is given in Table I for our representative highest precision points; all points calculated at less computational expense reflect the given results. The law expected in a massless phase from conformal field theory is

\[
\langle \phi(x)\phi(y) \rangle = \frac{C}{|x-y|^{2\bar{h}}}
\]

for conformal weight $h = \bar{h}$. We observe therefore a decay of the string order to zero in the thermodynamic limit in the intermediate phase, following a typical decay law of a massless phase, which we identify as a XY phase. It can also be observed that the exponent $\alpha$ decreases with increasing $J^z$ and increases with increasing $D$.

V. CONCLUSION

In our opinion, our numerical findings together with the analysis of Nomura and Kitazawa\cite{22} show that the emergence of the classical limit is governed by the third scenario of an almost classical phase diagram for $S = 2$ (Figure 6).

Why the failure of the AKLT model to account for the phase diagram of the $S = 2$ (and thus $S \geq 2$) phase diagram under the introduction of anisotropies, while it is extremely successful both for the isotropic Heisenberg model and for higher-$S$ spin chains with dimerization? In our view the failure is largely and simply due to the fact that the whole construction of the AKLT model(s) for various spin lengths $S$ resides entirely on the use of singlet spin-spin bonds. At the isotropic point, each of these singlet bonds is separated from the neglected triplets by an energy roughly of the order of the gap energy. Dimerization is rotationally invariant and accounted for by singlet redistribution between neighboring bonds. Anisotropies however destroy rotational invariance, splitting the triplet states, and lower the energetic distance between the singlet and the lowest triplet state(s). A description of the chain simply in terms of singlets then quickly becomes inadequate.

Obviously the $S = 1$ phase diagram has a very special property in that its XY and Haldane phases are separated by $J^z = 0$ strictly, which is linked to the fact that the $S = 1$ chain can be mapped to a six vertex times Ising model\cite{23}, a mapping which is not possible for higher spins. The $S = 2$ phase diagram reveals no such special property. It might therefore be conjectured that the $S = 1$ case itself is particular among integer spins and $S = 2$ the really generic case.
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TABLE I. Position of crossover from alternating to non-alternating sign behavior of the string order parameter for chain length $L$, $J^z = 1$, and on-site anisotropy $D$.

| $D$ | $L$=50 | $L$=100 | $L$=150 | $L$=200 |
|-----|--------|--------|--------|--------|
| 0.00 | –      | –      | –      | –      |
| 0.01 | –      | –      | –      | –      |
| 0.02 | –      | –      | 63     | 59     |
| 0.03 | –      | 41     | 39     | 35     |
| 0.04 | –      | 29     | 29     | 27     |
| 0.05 | 27     | 23     | 23     | 23     |
| 0.06 | 21     | 19     | 19     | 19     |
| 0.07 | 17     | 17     | 17     | 15     |
| 0.08 | 15     | 15     | 15     | 13     |
| 0.09 | 13     | 13     | 13     | 13     |
| 0.10 | 11     | 11     | 11     | 11     |

TABLE II. Exponent of string order power law decay for various values of $J^z$ and $D$, extracted from chains of length $L = 600$, keeping $M = 400$ DMRG block states.

| $J^z$ | $D$ | $\alpha$ |
|------|-----|----------|
| 1.0  | 1.5 | 1.24     |
| 1.8  | 1.5 | 1.14     |
| 2.5  | 2.3 | 0.99     |
| 2.7  | 2.4 | 1.00     |
| 2.7  | 2.7 | 1.04     |
| 3.0  | 2.7 | 0.95     |
| 3.3  | 2.8 | 0.86     |
| 3.3  | 3.0 | 0.90     |
| 4.2  | 3.6 | 0.95     |