LOW-DIMENSIONAL SPIN SYSTEMS: HIDDEN SYMMETRIES, CONFORMAL FIELD THEORIES AND NUMERICAL CHECKS

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Abstract:

We review here some general properties of antiferromagnetic Heisenberg spin chains, emphasizing and discussing the rôle of hidden symmetries in the classification of the various phases of the models. We present also some recent results that have been obtained with a combined use of Conformal Field Theory and of numerical Density Matrix Renormalization Group techniques.

1 Introduction and Summary.

For quite some time low-dimensional magnetic systems (i.e. (quantum) spins on 1D and/or 2D lattices) have been considered essentially only as interesting models in Statistical Mechanics with no realistic counterpart. It is only in recent times that systems that can be considered to a high degree of accuracy as assemblies of isolated or almost isolated spin chains and/or of spin ladders (a few chains coupled together) have began to be produced and have hence become experimentally accessible, thus renewing the interest in their study, which is by now one of the most active fields of experimental and theoretical research in Condensed Matter Physics.

In this paper we will discuss only some relevant properties of isolated spin chains, referring to the literature [15] for a general review of the properties of spin ladders.

More than one decade ago it was pointed out [20, 31] that integer spin chains (more specifically, spin-1 chains, but extensions to different values of the spin have also been devised in the literature [43]) possess unexpected and highly non-trivial hidden symmetries, whose spontaneous breaking manifests itself through the appearance of unusual and highly nonlocal "string" order parameters. The string order parameters, together with the more conventional magnetic order
parameters, can be used to classify the various phases that the phase diagram of one-dimensional magnets can display.

In the present paper, which is a slightly enlarged version of the talk presented by one of us (G.M.) at the \textit{XIII}th Conference on "\textit{Symmetries in Physics}"\footnote{The Conference, organized by Prof. B. Gruber, was held in Schloss Mehrerau in Bregenz (Voralberg, Austria), in the period 21-24 July, 2003.}, we will concentrate, without pretensions to full generality, on the discussion of a few models of antiferromagnetic Heisenberg chains, of their phase diagrams and on the rôle of hidden symmetries in their explanation. The paper is organized as follows. In Sect.2 we review some general facts concerning Heisenberg spin chains and discuss how in the continuum limit one can map a "standard" (see below for the terminology) Heisenberg chain onto an effective field theory described by a nonlinear sigma-model, and how the presence in the latter of a topological term can account for the radically different behaviors of integer versus half-odd-integer spin chains. In Sect.3, concentrating on spin-1 chains, we consider the effects of the addition to the "standard" model of biquadratic exchange terms and/or of Ising-like as well as of single-ion anisotropies, and how the addition of such terms can drive the model away from what is commonly called the "Haldane phase" (again, see below for an explanation) towards other phases. In this context we will introduce in a more explicit manner the notion of hidden symmetries and discuss their rôle. Sects.4 and 5 will be devoted to the discussion of more recent results that have been obtained by some of us \cite{17} with a careful and combined use of analytical (effective actions and Conformal Field Theory) and numerical (Density Matrix Renormalization Group) techniques. The final Sect.6 is devoted to the conclusions and to some general comments.

2 General Features of Spin Chains.

Let us begin by discussing here what can be considered as the "standard" model of an isotropic antiferromagnetic (\textit{AFM}) Heisenberg chain with nearest-neighbor (\textit{nn}) interactions, which is described by the Hamiltonian:

\begin{equation}
\mathcal{H} = J \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1} \equiv \mathcal{H}_\perp + \mathcal{H}_z \tag{1}
\end{equation}

\begin{equation}
\mathcal{H}_\perp = \frac{1}{2} J_\perp \sum_{i=1}^{N} \{ S^+_i S^-_{i+1} + S^-_i S^+_{i+1} \}; \quad \mathcal{H}_z = J_z \sum_{i=1}^{N} S^z_i S^z_{i+1}; \quad J_\perp = J_z = J \tag{2}
\end{equation}

where, for each $i = 1, \ldots, N$, $\vec{S}_i$ is a spin operator\footnote{\textit{and}: $S^\pm_i = S^x_i \pm i S^y_i$.}:

\begin{equation}
[S^\alpha_i, S^\beta_j] = i \hbar \delta_{ij} \varepsilon^{\alpha\beta\gamma} S^\gamma_i; \quad \alpha, \beta, \gamma = x, y, z; \quad \vec{S}_i^2 = \hbar^2 S(S+1) \tag{3}
\end{equation}

($S$ integer or half-odd integer) located at the $i$-th site of a one-dimensional lattice of $N$ sites, interacting with its neighbors with an AFM ($J > 0$) \textit{nn} interaction of strength $J$. Later on we will consider more general models in which $J_\perp \neq J_z$ will be allowed\footnote{$J_\perp = 0$, in particular, corresponds to the one-dimensional Ising model, a trivially soluble \textit{classical} model. Notice however that an Ising model in a \textit{transverse} magnetic field becomes a genuinely quantum and nontrivial model.}.
It may be useful to define a vector $\vec{n}_i$ as: $\vec{n}_i =: \vec{S}_i / \hbar S$, whereby:

$$\left[ n^\alpha_i, n^\beta_j \right] = i S^{\alpha \beta \gamma} n^\gamma_i; \quad \vec{n}_i^2 = 1 + \frac{1}{S}$$  \hspace{1cm} (4)

Although one is ultimately interested in the thermodynamic ($N \to \infty$) limit, for finite $N$ one can adopt either periodic boundary conditions (PBC’s), by imposing:

$$\vec{S}_{i+N} = \vec{S}_i \forall i$$  \hspace{1cm} (5)

by which the system is actually considered to "live" on a circle, or open boundary conditions (OBC’s), where $\vec{S}_1$ is coupled only to $\vec{S}_2$ and $\vec{S}_N$ only to $\vec{S}_{N-1}$.

The Hamiltonian of Eq.(1) has an obvious (global) $O(3)$ symmetry and, for PBC’s, it is also invariant under the (discrete) translation group of the lattice.

In the classical limit ($\hbar \to 0$ and $S \to \infty$ with: $\hbar S = \text{const.}$) the spins (the $\vec{n}_i$’s) become (see Eq.(4)) classical vectors (and $\vec{n}_i \in \mathbb{S}^2$, the unit sphere in $\mathbb{R}^3$). The minimum-energy configuration of the spins corresponds to: $\vec{n}_i \cdot \vec{n}_{i+1} = \text{const.} = -1$. Neighboring spins are then aligned antiparallel to each other and, in the absence of any external magnetic field, can point in a common but otherwise arbitrary direction on the sphere. This is the Néel state. Let us remark that, at variance with the ferromagnetic ($J < 0$) case, in which neighboring spins are all aligned parallel, at the quantum level the Néel state is not an eigenstate of the Hamiltonian (1). This points to the fact that quantum fluctuations will play a much more relevant rôle in the (quantum) antiferromagnetic case than in the ferromagnetic one.

The classical energy of the Néel state is of course: $E_N = -JN(hS)^2$. In this state the $O(3)$ symmetry is spontaneously broken down to $O(2)$, and the state exhibits long-range order (LRO).

Elementary excitations over the Néel state are well-known to be in the form of spin waves [38]: coherent deviations of the spins with a dispersion: $\omega(k) \propto k$ in the long-wavelength limit ($ka \ll 1$, with $a$ the lattice spacing). Hence, the (classical) spectrum of the Hamiltonian (1) is gapless. We would like to stress that nothing of what has been said hitherto depends on the value of the spin. At the classical level, the spin $S$ can be simply reabsorbed into a redefinition of the coupling constant ($J \to J(hS)^2$) and will contribute only an essentially irrelevant and additional multiplicative overall scale factor.

All this is elementary and well known. Let us turn now to the quantum case.

In the early 30’s Bethe [8] and Hulthen [30], employing what has been known since as the "Bethe-Ansatz", were able to show that the quantum $S = 1/2$ Heisenberg chain is actually an integrable model. We will not discuss here the Bethe-Ansatz in any detail [38], but will only summarize the main features of the solution of the $S = 1/2$ model. The (exact) ground state is nondegenerate, it exhibits only short-range AFM correlations, but no LRO. Parenthetically,

4 In which case the Hamiltonian should be actually rewritten as: $\mathcal{H} = J \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1}$.

5 Translational symmetry, if present is also broken, as the Néel state is not invariant under translations of a lattice spacing as the original Hamiltonian but only of twice the lattice spacing. This has important consequences on the location of the Goldstone mode [4, 40, 55] in momentum space, that we will not discuss here, however.

6 Or better $hS$.

7 From now on we will set for simplicity $h = 1$. 

3
this is in agreement with a general, and later, theorem [14]. The (staggered) static spin-spin correlation functions:

$$G^\alpha(i-j) = (-1)^{|i-j|} \langle S_i^\alpha S_j^\alpha \rangle; \alpha = x, y, z$$  \hspace{1cm} (6)

where \(\langle \ldots \rangle\) stands for the expectation value in the ground state, are all equal and decay algebraically to zero at large distances. We recall here that genuine LRO would imply (we omit here the index \(\alpha\)):

$$\lim_{|i-j| \to \infty} G(i-j) = O_N \neq 0$$  \hspace{1cm} (7)

this defining the Néel order parameter \(O_N\) (actually the square of the equilibrium staggered (i.e. sublattice) magnetization). On the other extreme, an exponential decay of the correlations of the form, say:

$$G(i-j) \approx \exp\{-|i-j|/\xi\} P(|i-j|)$$  \hspace{1cm} (8)

with \(P(.)\) some inverse power of \(|i-j|\) would imply a finite correlation length \(\xi\) and a mass gap (or, better, a spin gap) \(\Delta\) in the excitation spectrum roughly given by: \(\Delta \propto c\xi^{-1}\), with \(c\) a typical spin-wave velocity. Algebraic decay of correlations (formally corresponding to \(\xi \to \infty\)) implies then that the system is gapless. Summarizing, the main features of the \(S = 1/2\) Heisenberg AFM chain are that it has a (quantum) disordered ground state, with only short-range AFM correlations, and that it is gapless. It is therefore a (actually the first) prototype of a (quantum disordered and) quantum critical system [48]. It can be said then that, as compared with the classical limit, the system remains gapless but quantum fluctuations destroy LRO.

About thirty years later Lieb, Schutz and Mattis [36] (LSM) proved an important theorem stating that an \(S = 1/2\) chain has either a degenerate ground state or is gapless. No surprise that the Bethe solution obeys the Lieb-Schutz-Mattis theorem, which is however of much wider reach, as it can cover models that are more general than the "standard" \(nn\) chain, such as, e.g., the Majumdar-Ghosh [37] model, another integrable model that we will nor discuss here, though. The results of LSM were extended later on by other authors [3] beyond \(S = 1/2\) to cover all the half-odd-integer values of the spin. One can then take as rigorously proven that (at \(T = 0\)) isotropic half-odd-integer Heisenberg chains (with constant \(nn\) interactions) are all quantum disordered and quantum critical (i.e. gapless). This result was thought for quite some time to be "generic", i.e. valid for chains of arbitrary spin until, in the early 80’s, Haldane [28] put forward what has become known since as "Haldane’s conjecture", according to which half-odd-integer spin chains should be quantum disordered and gapless but integer spin chains should instead exhibit a spin gap and an exponential decay of correlations. This implied that, contrary to what happens in the classical limit, the physical behavior of spin chains should be a highly discontinuous function of the value of the spin.

Completely rigorous proofs of (the second part of) Haldane’s conjecture are still lacking. However, strong support to it comes from the analysis of the continuum limit of the Heisenberg chain, which we will briefly describe now, referring to the existing literature [1, 6, 23] for more details.
The canonical partition function for the Hamiltonian of Eq.(1) at temperature \( T = (k_B\beta)^{-1} \) (with \( k_B \) the Boltzmann constant):

\[
\mathcal{Z} = Tr \{ \exp [-\beta H] \}
\]

(9)
can be written as a spin coherent-state path-integral [32], whereby the spin variables get replaced, inside the path-integral, by classical variables according to:

\[
\vec{S}_i \rightarrow S \hat{\Omega}_i
\]

(10)
with \( \hat{\Omega}_i \) a classical unit vector: \(|\hat{\Omega}_i| = 1\). The next (and perhaps the most important) step in Haldane’s analysis is the parametrization of the \( \hat{\Omega}_i \)’s as:

\[
\hat{\Omega}_i = (-1)^i \hat{n}_i \sqrt{1 - \left(\frac{\vec{T}_i}{S}\right)^2 + \frac{\vec{T}_i}{S}}
\]

(11)
with: \(|\hat{n}_i| = 1\) and: \( \vec{n}_i \cdot \vec{l}_i = 0 \). The \( \hat{n}_i \)’s are assumed to be slowly-varying (on the scale of the lattice spacing). In this way, capitalizing, so-to-speak, on the information gained from the Bethe-Ansatz solution of the \( S = 1/2 \) model, they incorporate the information that the system still retains some short-range AFM ordering, which would be global only for \( \hat{n}_i = \text{const.} \) (and \( \vec{T}_i = 0 \)). The \( \vec{T}_i \)’s can be shown [1] to be the (local) generators of angular momentum. In the semiclassical (large \( S \)) limit, an expansion of the action in the path-integral up to lowest (second) order in the \( \vec{T}_i \)’s is justified. Taking then the continuum limit together with a gradient expansion, and integrating out the \( \vec{T}_i \)’s, one ends up with the following expression for the partition function:

\[
\mathcal{Z} = \int [D\hat{n}] \delta (\hat{n}_i^2 - 1) \exp \{-S_E - iS_B\}
\]

(12)
where \([D\hat{n}]\) stands for the functional measure and the \( \delta \) inside the integral is a functional \( \delta \). The first term in the action is given by:

\[
S_E = \frac{L}{\beta} \int_0^\beta dx \int_0^\beta d\tau \left\{ \frac{1}{2g} \left[ \frac{1}{c} |\partial_\tau \hat{n}|^2 + c |\partial_x \hat{n}|^2 \right] \right\}; \hat{n} = \hat{n}(x, \tau)
\]

(13)
where \( L (= N \times \text{lattice spacing}) \) is the length of the chain, \( g = 2/S \) is the coupling constant and: \( c = 2JS \) is the spin-wave velocity. This is simply the Euclidean action of an \( O(3) \) nonlinear sigma model [6, 23, 59] \((NL\sigma M)\). The second term is the integral of a Berry phase [50], and is given by:

\[
S_B = \frac{\theta}{4\pi} \int_0^L dc \int_0^\beta d\tau \hat{n} \cdot (\partial_\tau \hat{n} \times \partial_x \hat{n})
\]

(14)
with: \( \theta = 2\pi S \). The coefficient of \( \theta \) is easily recognized to be the Pontrjagin index [11, 41, 44], or winding number, of the map:

\[
\hat{n} : \mathbb{R}^2_{\text{comp}} \rightarrow S^2
\]

(15)

8This is what is known in the literature as “Haldane’s mapping.”
from spacetime compactified to a sphere and the two-sphere where \( \hat{n} \) takes values, and it is an integer: \( S_B \) is therefore a topological term, and: \( S_B = 2\pi n S \), \( n \in \mathbb{Z} \). Therefore, \( \exp \{-iS_B\} = 1 \) for integer \( S \) \( (\theta = 0 \mod (2\pi)) \), but: \( \exp \{-iS_B\} = (-1)^n (\theta = \pi \mod (2\pi)) \) if the spin is half-odd integer. This will generate interference between the different topological sectors, and it is the at the heart of the different behaviors of the two types of chains.

The pure \( (\theta = 0 \text{ in our case}) \) \((1 + 1) \) O(3) NLσM \( \) is a completely integrable model [60]. It has a unique ground state, and the excitation spectrum is exhausted by a degenerate triplet of massive excitations that are separated from the ground state by a finite gap. On the contrary, the \( \theta = \pi \) model was shown [45] to be gapless. Therefore, Haldane’s conjecture is fully confirmed by the analysis of the continuum limit of the Heisenberg model.

We would like only to mention in passing that quite a similar behavior occurs in spin ladders [15, 19, 46], namely even-legged ladders are gapped, while odd-legged ladders are gapped for integer spin and gapless for half-odd-integer spin. This “even-odd” effect has been shown [19, 51] to have the same topological origin an in single chains.

How do these results compare with the gaplessness (irrespective of the value of \( S \)) of the \( S \to \infty \) classical limit? The answer resides in the dependence of the spin gap on \( S \). Already at the mean-field level, but more accurately from large-\( N \) expansions and/or renormalization group analyses [42], it turns out that the spin gap \( \Delta \) behaves as: \( \Delta \propto \exp \{-\pi S \} \) for large \( S \) \( ^9 \). Hence, integer-spin chains become exponentially gapless for large \( S \), and the classical limit is recovered correctly.

\section{More general Models. Hidden Symmetries and String Order Parameters.}

In view of what has been said up to now, the second part of Haldane’s conjecture is by far the most intriguing part of it. Therefore integer spin chains are the most interesting ones, and we will concentrate from now on on \( S = 1 \) chains.

What has been called in the previous Section the ”standard” AFM Heisenberg model is actually a member of at least two larger families of models that we will illustrate briefly here. The first class of models, that we will call ”\( \theta-\)models”, includes a biquadratic term in the spins, and is described, setting \( J = 1 \), by the Hamiltonian:

\[ H = \sum_{i=1}^{N} \left\{ \cos \theta \left( \vec{S}_i \cdot \vec{S}_{i+1} \right) + \sin \theta \left( \vec{S}_i \cdot \vec{S}_{i+1} \right)^2 \right\} \]  

with \( \theta = 0 \) corresponding of course to the ”standard” model. Most of the phase diagram has been obtained [31] numerically, except for the points at \( \theta = \pm \pi/4 \), that correspond to integrable models. The point \( \theta = \pi/4 \) is the Sutherland model [53], while \( \theta = -\pi/4 \) is the integrable model [9, 54] of Babujian and Takhatajan\(^\text{10}\). Both models are gapless, while the entire region \(-\pi/4 < \theta < \pi/4 \) is known (numerically, again) to be gapfull. This whole region has been called

\(^9\Delta \propto \exp \{-\pi n S\} \) for spin ladders [19], where \( n_l \) is the number of legs of the ladder.

\(^\text{10}\)This point is also known familiarly as the ”Armenian point”.
the "Haldane phase". It includes a particularly interesting point that has been studied extensively by Affleck, Kennedy, Lieb and Tasaki [2] (AKLT), namely $\theta = \theta^*$, with: $\tan \theta^* = 1/3$. The corresponding Hamiltonian (omitting an irrelevant overall numerical factor) is given by:

$$H_{AKLT} = \sum_{i=1}^{N} \left\{ -\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \left( \vec{S}_i \cdot \vec{S}_{i+1} \right)^2 \right\}$$

(17)

This model is not completely integrable, but the ground state is known, it is unique in the thermodynamic limit and can be exhibited explicitly. The ultimate reason for this is that, apart from numerical constants, the $i$–th term in curly brackets is just:

$$-\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \left( \vec{S}_i \cdot \vec{S}_{i+1} \right)^2 = 2 \left[ P_2(i, i + 1) - \frac{1}{3} \right]$$

(18)

where $P_2(i, i + 1)$ is the projector [39] onto the state of total spin $S_{tot} = 2$ of the pair of $S = 1$ spins located at sites $i$ and $i + 1$. Therefore, the ground state of $H_{AKLT}$ must lie in the sector of the Hilbert space that is annihilated by all the projectors. It was shown by AKLT that the exact ground state (also called the "Valence-Bond-Solid" (VBS) state) can be constructed as a linear superposition of states $\Phi_{\sigma}$ that have the following characteristics. Let: $\sigma = \{\sigma_1, \ldots \sigma_N\}$ be a given spin configuration, with: $\sigma_i = 0, \pm 1, i = 1, \ldots, N$. Then, $\Phi_{\sigma}$ is such that:

i) $\vec{S}_i \Phi_{\sigma} = \sigma_i \Phi_{\sigma}$ and moreover: ii) If a given spin is, say, +1, then the next nonzero spin must be $-1$, and vice versa. Typical such states correspond therefore to spin configurations of the form:

$$\sigma = \{+00 -0 + -00 + \ldots\}$$

(19)

In other words, "up" and "down" spins do alternate in $\Phi_{\sigma}$, but their spatial distribution is completely random, as an arbitrary number of zeroes can be inserted between any two nonzero spins. So, if a given spin in nonzero, we can predict what the value of the next nonzero spin will be, but not where it will be located. There is therefore no long-range (Néel) order in any conventional sense in the VBS ground state, but a sort of "Liquid Néel Order" (LNO). Conventional Néel order would be characterized by a nonvanishing of (at least one of) the Néel order parameters:

$$O_N^\alpha = \lim_{|i-j| \to \infty} (-1)^{|i-j|} \langle S_i^\alpha S_j^\alpha \rangle; \ \alpha = x, y, z$$

(20)

In the VBS state and (numerically) in the whole of the Haldane phase one finds instead [2, 31]: $O_N^\alpha = 0, \alpha = x, y, z$, and this is consistent with the absence of a "rigid" Néel order.

There remains however what we have called the "liquid" Néel order, and it has been argued convincingly in the literature [20, 31] that this is connected with the nonvanishing of a novel class of order parameters that we will discuss now briefly. Let us begin by defining the string correlation functions as:

$$G_n^\alpha(n) = -\langle S_0^\alpha \exp \left[ i\pi \sum_{l=1}^{n-1} S_l^\alpha \right] S_n^\alpha \rangle; \ \alpha = x, y, z; \ n > 0$$

(21)
These are similar to the standard two-point correlation functions:

\[ G^\alpha(n) = (-1)^n \langle S_0^\alpha S_n^\alpha \rangle \tag{22} \]

whose asymptotic \((n \to \infty)\) limit yields the Néel order parameter(s), except that a \textit{string} of exponentials of intermediate spins has been inserted between the leftmost and the rightmost spins.

The \textit{string order parameters} \((\text{SOP's})\) \(O_S^\alpha\) are then defined as:

\[ O_S^\alpha = \lim_{n \to \infty} G_S^\alpha(n) \tag{23} \]

It turns out [2, 25] that the string correlation functions are strictly \textit{constant} in the \textit{AKLT} ground state, namely:

\[ G_S^\alpha(n) \equiv \text{const.} = O_S^\alpha = \frac{4}{9} \tag{24} \]

The ground-state spin-spin correlation functions have also been evaluated exactly for the \textit{VBS} state [2], and they turn out to be given by:

\[ G^\alpha(n) = \frac{4}{3} \left( \frac{1}{3} \right)^n \tag{25} \]

In other words: \(G^\alpha(n) \propto \exp \{-n/\xi_{\text{AKLT}}\}\), where the \textit{correlation length} \(\xi_{\text{AKLT}}\) is given, in units of the lattice spacing, by:

\[ \xi_{\text{AKLT}} = \frac{1}{\log 3} \simeq 0.91 \tag{26} \]

less than unity in units of the lattice spacing, implying a rather large spin gap.

So far for the ground state of the \textit{AKLT} model. String and ordinary correlation functions as well as Néel and string order parameters have also been evaluated (numerically away from the \textit{AKLT} point) for other points of the Haldane phase [25]. For example, at the Heisenberg point, exact diagonalization methods\(^\text{11}\) have shown that the string correlation functions are not strictly constant, but still decay exponentially to a value of the string order parameter that is somewhat smaller \((O_S^\alpha \simeq 0.36...)\) than the \textit{AKLT} value \((O_S^\alpha = 4/9 \simeq 0.44...)\) but still nonzero. The spin correlation length was also found [25] to be slightly larger than the \textit{AKLT} value, but still finite. So, there is convincing evidence that the entire Haldane phase is characterized by \textit{vanishing Néel order parameters} but by \textit{nonzero SOP's}. There is also convincing numerical evidence [25] that the string order parameters vanish at the integrable boundaries of the Haldane phase (i.e. for \(\theta = \pm \pi/4\)).

That the nonvanishing of the \textit{SOP's} is connected to the breaking of a symmetry, and hence to the onset of an ordering that is not apparent in the original Hamiltonian was clarified in a seminal paper by Kennedy and Tasaki [31] (\textit{KT}). With reference to a given configuration \(\{\sigma\}\), and defining \(N(\sigma)\) as the number of odd sites at which the spins are zero, one defines a new configuration \(\{\overline{\sigma}\}\) via:

\[ \overline{\sigma}_i = \exp \left[ \frac{i\pi}{N} \sum_{j=1}^{i-1} \sigma_j \right] \sigma_i \tag{27} \]

\(^{11}\text{With the Lanczos method and for chains with up to no more than 14 sites.}\)
and then a unitary operator $U$ via:

$$U \Phi_\sigma = (-1)^{N(\sigma)} \Phi_\sigma$$

(28)

In a nutshell, the action of $U$ amounts to leaving the first nonzero spin unchanged and to flipping every other nonzero spin proceeding to the right of the chain. For example:

$$\{+ + 0 + 00 + 0 - 0 + +\} \mapsto \{+ - 0 - 00 + 0 + 0 + -\}$$

$$\{0 + -00 + 00 + -00-\} \mapsto \{0 + +00 + 00 + +00+\}$$

(29)

and so on. It is obvious that $U$ is a unitary. What is less obvious is that the unitary transformation is a nonlocal one, in the sense that $U$ cannot be written as a product of unitary operators acting at each single site. This has the important consequence that symmetries that are local (in the above sense) for the Hamiltonian $H$ will of course remain symmetries of the transformed Hamiltonian $\tilde{H}$ (as $U$ is unitary) but need not survive as local symmetries of $H$. Specifically, the symmetry group of $H$ is $SU(2)$, that includes a discrete $Z_2 \times Z_2$ subgroup of rotations of $\pi$ around the coordinate axes. Explicitly, the transformed Hamiltonian has the form [31]:

$$\tilde{H} = \sum_i \{ \cos \theta h_i + \sin \theta (h_i^2) \}$$

(30)

where:

$$h_i = -S_i^x S_{i+1}^x + S_i^y \exp \{ i \pi (S_i^z + S_{i+1}^z) \} S_{i+1}^y - S_i^z S_{i+1}^z$$

(31)

and it evident that $Z_2 \times Z_2$ is the only local surviving symmetry group of the transformed Hamiltonian $\tilde{H}$. Even more important is how the string order parameters transform. The result is [31]:

$$O_\alpha (H) = O_{f\text{erro}}^\alpha (\tilde{H})$$

(32)

where:

$$O_{f\text{erro}}^\alpha (\tilde{H}) = \lim_{|i-j| \to \infty} \langle S_i^\alpha S_j^\alpha \rangle |\tilde{H}\rangle$$

(33)

and the r.h.s stands here for an average taken w.r.t. the ground state of the transformed Hamiltonian. The transformed order parameter is now a ferromagnetic order parameter. Therefore: $O_\alpha^S (H) \neq 0 \Rightarrow O_{f\text{erro}}^\alpha (\tilde{H}) \neq 0$, and this implies the onset of a spontaneous ferromagnetic polarization in the $\alpha$-th direction in the ground state of $\tilde{H}$. This in turns entails a partial (if $O_{f\text{erro}}^\alpha (\tilde{H}) \neq 0$ for just one value of $\alpha$) or total (if this happens in more than one direction) spontaneous breaking of the discrete $Z_2 \times Z_2$ symmetry. It is known [4, 55] that spontaneous breaking of a continuous symmetry is accompanied by massless excitations (the Goldstone modes), while breaking of a discrete symmetry usually implies the opening of a gap (the most conspicuous and familiar example being the 2D Ising model). Therefore, $KT$ were led to consider the spontaneous breaking of the $Z_2 \times Z_2$ symmetry as the origin of the Haldane gap.

\[12^*\text{Notice also that: } N(\sigma) = N(\overline{\sigma}), \text{ as zero spins are mapped into zero spins.}\]
One has however to be a bit careful on this point. It appears to be true that spontaneous (partial or total) breaking of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry implies the generation of a spin gap. But:

i) The converse need not be true. We will see that there are spin models that exhibit *gapped* phases\(^\text{13}\) while retaining the full $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, and:

ii) The mere nonvanishing of (one or more) string order parameters is not enough to fully determine in which (gapped) phase the system is. It is the full set of order parameters, both string and Néel, that allows for a full characterization of the various phases. In particular, the Haldane phase is fully characterized by the vanishing of all the Néel order parameters and by all the three string parameters being nonzero.

We turn now to a different class of models, the so-called "\(\lambda - D\)" family of models\(^\text{14}\). They are described by the family of Hamiltonians (parametrized by two real parameters, \(\lambda\) and \(D\)):

$$
\mathcal{H} = \sum_{i=1}^{N} \left\{ S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D (S_i^z)^2 \right\}
$$

(34)

The "standard" (isotropic) AFM Heisenberg model corresponds of course to \(\lambda = 1\) and \(D = 0\). \(\lambda = -1\) (and \(D = 0\)) can be easily shown\(^\text{15}\) to correspond to a (isotropic) ferromagnetic Heisenberg model. \(|\lambda| \neq 1\) introduces an "Ising-like" anisotropy, while \(D \neq 0\) introduces what is called "single-ion" anisotropy.

The model can be solved exactly for \(S = 1/2\) \(^{33}\), but no exact solutions are available for integer spin. There are obvious asymptotic limits when either \(\lambda\) (resp. \(D\)) is large and \(D\) (resp. \(\lambda\)) not too large, so that the "\(\lambda\)-term" (resp. "\(D\)-term") can be considered as a zeroth-order Hamiltonian and the rest as a perturbation:

i) \(|\lambda| \gg 1\). The reference ground state is either a Néel AFM state (\(\lambda > 0\)) or a ferromagnetic (\(\lambda < 0\)) state.

ii) \(|D| \gg 1\). For \(D > 0\) (the so-called "large-\(D\)" phase) the reference state becomes a planar state with \(S_i^z = 0\) for all \(i\)'s, while for \(D < 0\) the reference state is a state where \(S_i^z = 0\) is excluded, hence a state where the \(S = 1\) spins become effectively two-level systems, and a detailed map of the model into an effective spin-1/2 model \(17, 47\) can be successfully performed. For \(|\lambda| \neq 1\) and \(D \neq 0\) the symmetry group of the Hamiltonian is \(O(2) \times \mathbb{Z}_2\) (the \(\mathbb{Z}_2\) factor corresponding to a reflection in the \(x - y\) plane: \(S_i^z \rightarrow -S_i^z\)).

Apart from these limiting cases, the model has been studied analytically \(49\) as well as numerically \(10, 13, 26, 52\), and the corresponding phase diagram is displayed in Fig.1.

The various sectors of the phase diagram can be characterized as follows \(13, 17, 22\):

i) the Haldane phase. The ground state is unique with total component \(S_{\text{tot}}^z = 0\) of the spin. The order parameters are: \(O_N^\alpha = 0\), \(O_N^z \neq 0\), \(\alpha = x, y, z\). The (Haldane) gaps are in different spin channels according to the sign of \(D\), but nonzero in any case. The isotropic, Heisenberg point \(\lambda = 1, D = 0\) is in this

\(^{13}\)The so-called "large-\(D\)" phases of the "\(\lambda - D\)" model to be discussed immediately below.

\(^{14}\)This is the class of models on which the Bologna group is currently working.

\(^{15}\)By performing a rotation of \(\pi\) around the \(z\)-axis on one of the two sublattices (i.e. on every other site).

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phase, and lies on a line separating the two subphases, that are denoted as $H1$ and $H2$ in the literature [10].

ii) The Néel phase. The ground state is doubly degenerate, and the order parameters are: $O^\alpha_N = O^\alpha_S = 0$ for $\alpha = x, y$, but: $O^z_N, O^z_S \neq 0$.

iii) The large-$D$ phase. The ground state is unique, it is gapped, but here: $O^\alpha_S = O^\alpha_N = 0 \forall \alpha$.

iv) The two XY phases. These are both gapless phases. They are distinguished by the nature of the low-lying spin excitations (spin-1 in the XY1 phase, spin-2 in the XY2 phase).

v) The ferromagnetic phase. The ground state is doubly degenerate, with maximal magnetization: $S^z_{\text{tot}} = \pm N$, and the phase is gapped. In this case it is the ferromagnetic order parameter that is nonvanishing, and actually [16]: $O_f = 1$ (the other two being zero). Also: $O^z_S(j,k) = (-)^{j-k-1}$, while: $O^x,y_S = 0$.

Anticipating some of the numerical results of Sect.5, we give below, in Figs.2 and 3, some examples [16] of the behavior of the various correlators and order parameters as functions of the parameters of the model.

Concerning the nature of the transitions between the various phases [10, 13, 17], both the Haldane-large-$D$ and the Haldane-Néel transition lines are critical (gapless) lines. The two critical lines merge at a tricritical point (at $D \simeq \lambda \simeq 3$), above which the Haldane phase disappears and the transition (a large-$D$-Néel transition, now) is first-order. The XY-ferromagnetic transition is instead a first-order one, as well as the large-$D$-ferromagnetic transition. Finally, The Haldane-XY transition is considered [13] to be of the Berezinskii-Kosterlitz-Thouless [7, 34] (BKT) type, as well as the XY-large-$D$ transition.
Figure 2: Ordinary and string correlation functions in the Haldane phase: (a) $G_z(k)$, (b) $\frac{1}{2}(-)^k(S^z_k S^-_{-k})$, (c) $G^x_z(k)$ and (d) $G^x_S(k)$. Selected values of the parameters are $(D = 0.5, \lambda = 1)$. Note that with this choice the transverse correlation length is appreciably larger than the longitudinal one. The data have been obtained with finite-size DMRG on a chain of $L = 100$ spins ($S = 1$) with $PBC$ and $M = 216$ states (Sect. 5 for details).

The "\(\lambda - D\)" model has also been studied by KT. Applying the same nonlocal unitary transformation that was discussed previously, they showed that the transformed Hamiltonian, whose explicit form we will not give here, is still given in terms of the operators $h_i$ (see Eq. (31)), and retains therefore $Z_2 \times Z_2$ as the only local symmetry, just as in the case of the Hamiltonian of Eq. (16). Therefore, the same conclusions as before apply concerning the connection of the nonvanishing of the string order parameters with the spontaneous breaking of the $Z_2 \times Z_2$ symmetry.

In the present paper we will address mainly to the detailed nature of the Haldane-large-\(D\) and Haldane-Néel critical transition lines. It is known that the (large distance) critical behavior of one-dimensional quantum systems is well described by Conformal Field Theory [12, 21, 24, 27, 33] (CFT). In the next Section we will report on a proposal of an effective CFT for the "\(\lambda - D\)" model on the Haldane-large-\(D\) critical line. This allows for the prediction of the operator content of the theory, and hence also for the prediction of the structure of the conformal tower of excited states above the ground state. To confirm the predictions, we will report also on extended numerical analyses, whose details will be reported elsewhere [18], that fully confirm the theoretical predictions.

4 Conformal Field Theory and Effective Actions.

Let us begin by recalling some basic results and examples of CFT that will be used in the forthcoming analysis of the critical properties of the spin-1 $\lambda - D$ chain.

It is well known [21, 27] that critical properties of two-dimensional systems
are completely classified by $CFT$'s: since in $2D$ the conformal group is infinite dimensional, the Hilbert space of a conformally invariant theory can be completely understood in terms of the irreducible representations of its algebra, the Virasoro algebra. We recall that the latter has an infinite number of generators, denoted with $L_n, \bar{L}_n$ ($n \in \mathbb{Z}$) for its holomorphic and antiholomorphic part respectively, satisfying the commutation relations:

$$[L_n, L_m] = (m - n)L_{m+n} + \frac{c}{12}(m^3 - m)\delta_{m+n,0}$$

and similarly for the $\bar{L}_n$. The constant $c$ is called the central charge of the algebra or the conformal anomaly. Since we are interested in a comparison between theoretical predictions and numerical data, which are performed on a finite lattice, we will consider a $CFT$ defined on a cylinder with spatial dimension of finite length $L$. In this case [12, 21], the energy and the momentum operator are represented respectively by:

$$H = \frac{2\pi}{L} \left( L_0 + \bar{L}_0 - \frac{c}{12} \right)$$
$$P = \frac{2\pi}{L} (L_0 - \bar{L}_0)$$

In order for $H$ to be bounded from below, we must restrict our attention to highest weight representations of the Virasoro algebra, for which there exists a highest weight (or primary) state $|\Delta, \bar{\Delta}\rangle$ satisfying:

$$L_0|\Delta, \bar{\Delta}\rangle = \Delta|\Delta, \bar{\Delta}\rangle , \quad L_n|\Delta, \bar{\Delta}\rangle = 0 \quad \text{for} \ n > 0$$
and analogous relations with respect to the $\vec{L}_n$ generators.

Each of these representations is thus identified by the values of the central charge $c$ and of the couple $(\Delta, \bar{\Delta})$ (the conformal dimensions). They fix both the energy and the momentum of the primary state $|\Delta, \bar{\Delta}\rangle$, according to:

$$E^0_{\Delta, \bar{\Delta}} = \frac{2\pi}{L} (\Delta + \bar{\Delta} - \frac{c}{12})$$  \hspace{1cm} (39)

$$P^0_{\Delta, \bar{\Delta}} = \frac{2\pi}{L} (\Delta - \bar{\Delta})$$  \hspace{1cm} (40)

Notice that, in a finite geometry (with $P_{BC}$), the vacuum state, corresponding to $\Delta = \bar{\Delta} = 0$, has a non-zero energy (Casimir effect):

$$E^0_\text{vac} = -\frac{\pi c}{6L}$$  \hspace{1cm} (41)

Also, the two-point correlation function of the operator creating a given primary state out of the vacuum ($|\Delta, \bar{\Delta}\rangle = \mathcal{O}_{\Delta, \bar{\Delta}}(0)$) has an algebraic decay whose critical exponents are determined by the values of the conformal dimensions $(\Delta, \bar{\Delta})$: one has [21, 27]

$$\langle \mathcal{O}_{\Delta, \bar{\Delta}}(z, \bar{z}) \mathcal{O}_{\Delta, \bar{\Delta}}(0, 0) \rangle \propto \frac{1}{z^{2\Delta} \bar{z}^{2\bar{\Delta}}}$$  \hspace{1cm} (42)

Finally, from the primary state $|\Delta, \bar{\Delta}\rangle$ one can obtain all excited (or secondary) states by applying strings of powers of $L_n, \bar{L}_n$ with $n < 0$. It is easy to see that, if $m, n < 0$, the commutation relations (35) imply: $L_0(L_m)^j|\Delta, \bar{\Delta}\rangle = (\Delta + mj)|\Delta, \bar{\Delta}\rangle, \bar{L}_0(\bar{L}_n)^k|\Delta, \bar{\Delta}\rangle = (\bar{\Delta} + nk)|\Delta, \bar{\Delta}\rangle$, so that the secondary states have energies and momenta:

$$E^{(r, \bar{r})}_{\Delta, \bar{\Delta}} - E^0_\text{vac} = \frac{2\pi}{L} (\Delta + \bar{\Delta} + r + \bar{r})$$  \hspace{1cm} (43)

$$P^{(r, \bar{r})}_{\Delta, \bar{\Delta}} = \frac{2\pi}{L} (\Delta - \bar{\Delta} + r - \bar{r})$$  \hspace{1cm} (44)

with $r, \bar{r} \in \mathbb{N}$ and a degeneracy that can be explicitly calculated for each representation. It may happen that some of these states have null norms. In this case the true (non-degenerate) Hilbert space of states is obtained after projecting out these null vectors, which therefore do not contribute to the operator content of the corresponding CFT. The quantity in brackets in the right hand side of Eq. (43) yields the coefficients with which the energy of the corresponding state scales to zero in the thermodynamic limit. It is therefore called "scaling dimension" and will be denoted by $d^{(r, \bar{r})}_{\Delta, \bar{\Delta}}$ in the sequel.

Let us examine some examples. We will consider only unitary theories, corresponding [21] to the following two sets of values of the central charge $c$:

$$c = 1 - \frac{6}{p(p+1)}, \quad p = 3, 4, \ldots ;$$ \hspace{1cm} (45)

$$c \geq 1.$$ \hspace{1cm} (46)

The first set of values corresponds to the so-called minimal models [21, 27], whose primary states are of finite number. Their conformal dimensions are given by the formula:

$$\Delta_{rs}, \bar{\Delta}_{rs} = \frac{[(p+1) r - ps]^2 - 1}{4p(p+1)}, \quad 1 \leq s \leq r \leq p - 1, \quad r, s \in \mathbb{Z}$$  \hspace{1cm} (47)
Theories with $c \geq 1$ have instead an infinite number of primary states.

The simplest case of a CFT corresponds to $c = 1/2$ ($p = 3$ in Eq. (45)) and describes the universality class of the two-dimensional Ising model. According to (47), there are only three primary operators: the identity $I$ corresponding to the vacuum, $(\Delta, \bar{\Delta}) = (0, 0)$, the Ising spin $\sigma$ with $(\Delta, \bar{\Delta}) = (1/16, 1/16)$ and the energy density $\varepsilon$ with $(\Delta, \bar{\Delta}) = (1/2, 1/2)$. Notice that the spin-spin correlator $\langle \sigma(x) \sigma(0) \rangle$ decays with a critical exponent $\eta' = 4\Delta_\sigma = 0.25$. In Table 1 we list the lowest conformal (primary and secondary) states, together with their scaling dimensions and momenta. As explained in the next section, a comparison with the numerical data given in the last column will allow us to conclude that the Haldane-Néel critical transition line is indeed of the Ising type.

### Table 1: Columns 1-4 show the conformal dimensions $(\Delta, \bar{\Delta}), (r, \bar{r})$, the scaling dimensions $d^{(r, \bar{r})}_{\Delta, \bar{\Delta}}$ and the momenta $P^{(r, \bar{r})}_{\Delta, \bar{\Delta}}$ of the lowest conformal states in the $c = 1/2$ minimal model. The numerical results in the last column are explained in Sect. 5.

| $(\Delta, \bar{\Delta})$ | $(r, \bar{r})$ | $d^{(r, \bar{r})}_{\Delta, \bar{\Delta}}$ | $P^{(r, \bar{r})}_{\Delta, \bar{\Delta}}$ | $d_{(\text{num})}$ |
|-------------------------|----------------|-------------------------------|---------------------------------|------------------|
| $(0, 0)$; $(0, 0)$     |               | 0                             | 0                               | 0.1250 ± 0.0004  |
| $(1/16, 1/16)$; $(0, 0)$ | 1/8           | 0                             | $\pm 2\pi/L$                   | 1.0959 ± 0.0008  |
| $(1/2, 1/2)$; $(0, 0)$ | 1             | 0                             | $\pm 2\pi/L$                   | 1.100 ± 0.003    |
| $(1/16, 1/16)$; $(0, 0)$ | 9/8           | $\pm 2\pi/L$                 | 1.87 ± 0.02                    | 1.904 ± 0.004    |
| $(1/2, 1/2)$; $(0, 0)$ | 2             | $\pm 2\pi/L$                 | 1.87 ± 0.02                    | 1.86 ± 0.01      |
| $(0, 0)$; $(2, 0)$, $(0, 2)$ | 2             | $\pm 4\pi/L$                 |                                 |                  |

We discuss now briefly the $c = 1$ case, which exhibits a much richer structure. It corresponds to the field theory of a free compactified bosonic field, i.e. to a Gaussian model with Lagrangian:

$$
\mathcal{L} = \frac{1}{2} \left[ \frac{1}{v} (\partial_\nu \Theta)^2 + v (\partial_\nu \Theta)^2 \right]
$$

(48)

where $\Theta$ represents an angular variable spanning a circle of a given radius $R$ and the constant $v$, which has the dimension of a velocity, is called spin velocity. If we assume for $\Theta$, and hence for its dual field $\Phi$\textsuperscript{16}, periodic boundary conditions, the Hilbert space of the theory splits into a direct sum of distinct topological sectors labeled by the winding numbers $n, m \in \mathbb{Z}$ of the fields $\Theta$ and $\Phi$ respectively. The primary fields are then vertex operators of the form [21, 27]

$$
V_{mn} = \exp \left( i \sqrt{4\pi K} n \Phi + i \sqrt{\pi / K} m \Theta \right)
$$

(49)

whose scaling dimensions are given by

$$
d_{mn} = \left( \frac{m^2}{4K} + n^2 K \right), \quad K = \frac{\pi}{R^2}
$$

(50)

\textsuperscript{16}If we decompose the field $\Theta$ in its holomorphic and antiholomorphic part, $\Theta(z, \bar{z}) = \Theta_h(z) + \Theta_{ah}(\bar{z})$, the dual field is defined as $\Phi = \Theta_h(z) - \Theta_{ah}(\bar{z})$. 

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Notice that the latter depend explicitly on the radius of compactification. Thus we obtain a different $c = 1$ theory for each value of $R$, i.e. of $K$. For example, $K = 1$ corresponds (via fermionization [21, 27]) to a 1D model of free Dirac ($FD$) fermions. The $K = 1/2$ point is said to be self-dual ($SD$) since it is invariant under the duality transformation $\Theta \Leftrightarrow \Phi, m \Leftrightarrow n$, while the point $K = 2$ corresponds to the BKT critical theory. We remark also that the energy operator $(\partial \Theta)^2$ has conformal dimension 2 for any value of $R$ and hence it is always marginal. The effect of adding it to the Lagrangian (48) results only in a change of the coupling constant in front, which, in turn, can be absorbed into a rescaling of the radius of compactification of $\Theta$. Thus we generate a continuous line of inequivalent critical $c = 1$ theories, corresponding to different values of $K$.

It is well known [27] that the Gaussian model (48) describes the continuum limit of the spin 1/2 XXZ chain with anisotropy parameter $\Delta$, as long as $-1 \leq \Delta \leq 1$. From the exact Bethe-ansatz results, one can show [27] that the interesting cases $\Delta = -1, 0, 1$ correspond to the $SD$, $FD$ and $BKT$ points of the bosonic theory, respectively. We would like to show now, that the Gaussian model (48) describes also the critical properties of the spin-1 $\lambda - D$ Hamiltonian (34) on the Haldane-large-D transition line. In doing so, we will also establish a relationship between the coupling constants $D, \lambda$ of the discrete model and those of the continuum theory, namely the spin-wave velocity $v$ and the compactification radius. This will allow us to make quantitative theoretical predictions to be compared, in next section, to the numerical results.

In the spirit of Haldane’s mapping, we start from a classical solution, which for $D > \lambda - 1$, is a planar state where the unit vectors $\hat{\Omega}_j(\tau)$ that represent our spins $\vec{S}_j(\tau)$, see Sect.2) are Néel ordered in the $xy$-plane: $\hat{\Omega}_j(\tau) = (\cos(\theta_0 + j\pi), \sin(\theta_0 + j\pi), 0)$. Hence we make the Haldane-like ansatz:

$$\hat{\Omega}_j(\tau) = (-1)^j \hat{n}_j(\tau) \sqrt{1 - \frac{l_j^2(\tau)}{S^2}} + \hat{z} \frac{l_j(\tau)}{S}$$

where $\hat{n}_j(\tau) = e^{i\theta_j(\tau)} \in O(2)_{xy}$, $\hat{z}$ is the unitary vector $(0, 0, 1)$, and the fluctuation field $l_j$ is supposed to be small. Thus, as for the isotropic case, it is possible to obtain an effective Lagrangian that describes the low-energy physics of the Hamiltonian (34) in the continuum limit. Carrying out this calculation as explained in Sect.2, one obtains in this case a Gaussian model (48), where now $\Theta = \theta / \sqrt{g}$ and

$$g = \frac{1}{s} \sqrt{2(1 + D + \lambda)}; \quad v = s \sqrt{2(1 + D + \lambda)}$$

In other words, we have a free theory for a bosonic field $\Theta$, which is compactified along a circle of radius $1/\sqrt{g}$. Thus, the operator content of the theory can be read from Eq. (49): the list of primary operators is exhausted by the vertex operators $V_{mn}$ whose scaling dimensions are given by Eq. (50), with $K = \pi/g$.

In addition, the scaling dimensions (50) fix also the (non universal) critical exponents of the correlation functions. For instance it is easy to see that the transverse spin-spin correlator should decay according to:

$$\langle S^x(0)S^x(-x) \rangle \approx \langle e^{i\theta(0)} e^{-i\theta(-x)} \rangle \propto |x|^{-\eta} \text{ with } \eta = 2d_{10} = g/2\pi.$$

16
The Density Matrix Renormalization Group and Spin Chains.

The code that we have used for density matrix renormalization group (DMRG) calculations follows rather closely the algorithms reported in White's seminal papers [56, 57], with the following points to be mentioned:

• The superblock geometry was chosen to be $[B^s \bullet B^s_{\text{ref}} \bullet]$ with PBC, where $B^s_{\text{ref}}$ is the (left ↔ right) reflected of block $B^s$ with $s'$ sites. The rationale for adopting this configuration is that, being effectively on a ring, the two blocks are always separated by a single site, for which the operators are small matrices that are treated exactly (no truncation) [57]. In this way we expect a better precision in the correlation functions calculated fixing one of the two points on these sites and moving the other one along the block. Moreover, whenever the system has an underlying antiferromagnetic structure (typically when a staggered field is switched on), this geometry seems to be the one that preserve it at best, both for even and odd values of $s$.

• We used the finite-system algorithm with three iterations. This prescription should ensure the virtual elimination of the so-called environment error [35], which is expected to dominate in the very first iterations for $L < L^*(m)$ (see below). Normally the correlations are computed at the end of the third iteration, once that the best approximation of the ground state is available. This has the advantage of using less memory during the finite-size iterations but requires the storage of all the matrices needed to represent, on the reduced basis of the last step, the operators entering the correlation functions of interest. At the moment, disk storage is the ultimate factor that limits the size of the systems that we are able to treat.

• We always exploit the conservation of $S^z_{\text{tot}}$. With the exception of the ferromagnetic phase, that we do not address now, the ground state(s) is (are) at $S^z_{\text{tot}} = 0$ [10]. In order to maximize their accuracy, the correlations are calculated targeting only the lowest-energy state within this sector. However, in order to analyze the energy spectrum, we had to target also the lowest-energy states in the other sectors $|S^z_{\text{tot}}|=1,2,\ldots$ and/or a few excited states within the $S^z_{\text{tot}} = 0$ sector, depending on the phase of interest. On the one hand, this requires a modification of the basic Lanczos method to go beyond the lowest eigenvalue of the superblock Hamiltonian. On the other hand, once the $N_z$ eigenvalues of interest are found, one can build the block density matrix as the average (mixture) of the matrices associated with the corresponding $N_z$ eigenvectors. At present we are not aware of any specific "recipe" other than that of equal weights.

Going back to the modified Lanczos routine, our DMRG code implements the so-called Thick Restart algorithm of Wu and Simon [58]. Once $S^z_{\text{tot}}$ is fixed, in a given run we want to determine simultaneously the first $N_z$ levels $|S^z_{\text{tot}}; b\rangle$ with $b=0,1,2,\ldots,N_z-1$ (the ground state being identified by $(S^z_{\text{tot}} = 0, b = 0)$). Then, as in the conventional Lanczos scheme, we have to push the iteration until the norms of the residual vectors and/or the differences of the energies in consecutive steps are smaller than prescribed tolerances ($10^{-9} - 10^{-12}$ in our calculations). The delicate point to keep under control is that, once the lowest state $|S^z_{\text{tot}}; 0\rangle$ is found, if we keep iterating searching for higher levels the orthogonality of the basis may be lost, just because the eigenvectors corresponding to these levels
tend to overlap again with the vector $|S_{\text{tot}}^z; 0\rangle$. As a result, the procedure is computationally more demanding to the extent that one has to re-orthogonalize the basis from time to time. Typically, we have seen that this part takes a 10-20% of the total time spent in each call to the Lanczos routine. We have also observed that if this re-orthogonalization is not performed, one of the undesired effects is that the excited doublets (generally due to momentum degeneracy) are not correctly computed. More specifically, it seems that while the two energy values are nearly the same in the asymmetric stages of the iterations, when the superblock geometry becomes symmetric ($s = s'$ in the notations of the preceding point) the double degeneracy is suddenly lost and only one of the two states appears in the numerical spectrum.

So far for the specific algorithm. Now, the crucial point to consider in accurate DMRG calculations is the choice of $M$, that is, the number of optimized states. White argued [57] that the convergence of the ground state energy is almost exponential in $M$ with a step-like behaviour, probably related to the successive inclusion of more and more complete spin sectors. Unfortunately, the effective accuracy gets poorer when we deal with energy differences and correlation functions, for which little is known about convergence. It must be told, however, that despite its name the DMRG performs somehow better for systems with a definite gap rather than for gapless (critical) ones. We refer to the papers by Andersson, Boman and Östlund [5] and by Legeza and Fáth [35] where, for different systems and in terms of different observables, the following common feature emerges: Even if the quantum system is rigorously critical in the limit $L \to \infty$, the DMRG truncation introduces a spurious length, $L^*(m)$, which, as expected, diverges as $M$ is increased. (Our analysis of the accuracy of the energy levels in some selected points of the $\lambda - D$ chain near criticality leads to a similar conclusion [18]). Hence, even if we are technically able to deal with sizes $L > L^*(m)$ (at a given $M$), as far as criticality is concerned we cannot rely completely on the DMRG data because the system experiences an effective length which should be absent in the critical regime.

Therefore, our strategy can be summarised as follows: We fix a rather high value of $M$ such that the trustable values of $L$ are sufficiently large to see the scaling limit of CFT, but not too large as compared to $L^*(m)$. In other words, even in the study of (supposed) critical systems, we prefer to exploit the computing resources to include as many DMRG states as possible, and to refine the calculations with finite-size iterations, rather than trying to take naively the limit $L \to \infty$. In addition, to judge whether $M$ is sufficiently large or not we checked the properties of traslational and reflectional invariance that the correlation functions should have $^{17}$. To be specific, if $\mathcal{G}(0, k)$ is a certain correlation function computed starting at $j = 0$, we have always increased $M$ (at the expenses of $L$) until the bound $|\mathcal{G}(\ell, \ell \pm k) - \mathcal{G}(0, k)|/\mathcal{G}(0, k) \lesssim 0.05$ was met for $k$ varying from 0 to $\ell = L/2$, possibly with the exception of the ranges where $\mathcal{G}(0, k)$ is below numerical uncertainties ($10^{-6}$, say).

The quality of the numerical analysis of the critical properties depends heavily on the location of the critical points of interest. As far as the transitions from the Haldane phase are concerned, it is convenient to fix some representative values of $\lambda$ and let $D$ vary across the phase boundaries. This preliminary

$^{17}$In [18] it is shown that, in general, $\mathcal{G}^{x,y}_{S}(j, k)$ behaves nontrivially under $j \leftrightarrow k$, due to the fact that the ground state is not necessarily in the $S_{\text{tot}}^z = 0$ sector.
task of finding \( D_c(\lambda) \) turns out to be crucial for subsequent calculations and is divided in two steps. First, one has to get an approximate idea of the transition points using a direct extrapolation in \( 1/L \) of the numerical values of the gaps, computed at increasing \( L \) with a moderate number of DMRG states. Clearly, one may want to explore a rather large interval of values and so the increments in \( D \) will not be particularly small (0.1, say). Then, the analysis must be refined around the minima of the curves \( \Delta E \text{-vs-} D \) with smaller increments in \( D \) and a larger value of \( M \). In our problem, the approach that seems to give better results is standard finite-size scaling (FSS) theory [26, 29] (for instance as compared to the phenomenological renormalization group).

Once the critical point is located, we take full advantage of the conformal structure by looking at the finite-size spectrum (see Eqs. (41) and (44)) of relevant and marginal operators. In practice, we select a number of states that tend to become degenerate with the ground state and look for straight lines in the \( \Delta E \text{-vs-} L^{-1} \) plot. Then, from a best fit we expect to have a very small offset (ideally a zero gap in the thermodynamic limit) and a slope given by the scaling dimension \( d \) multiplied by the velocity prefactor, \( v \), which is absent in the field-theoretical formulation but has to be determined (in terms of the microscopic parameters) in a lattice system. In the latter case, Eq. (41) should contain also a term \( e_\infty L \), \( e_\infty \) being the energy density of the problem at hand.

Actually, due to the prefactor \( v \), we have to imagine a self-consistent procedure: Depending on the type of the transition we have in mind (that is, depending on the central charge \( c \)), we stick on one or more levels in the spectrum that have exactly \( d = 1 \). Then the slope of these is nothing but \( v \). Once the velocity is estimated, one uses Eq. (41) to best fit the product \( cv \) and see whether the value of \( c \) and the hypothesis on the universality class are self-consistent or not.

To clarify the matter, let us start with the simpler case of the Haldane-Néel transition, that is thought to be in the 2D Ising universality class. Fixing \( \lambda = 0.5 \) we find \( D_c(0.5) = -1.2 \), and the \( \beta \)-function method [29] yields \( \nu(0.5) = 1.023 \pm 0.009 \), as far as the gap exponent, \( \Delta E \propto (D - D_c)^\nu \) is concerned. Moreover, we observe the following nontrivial feature of the spectrum: The massless modes described by the CFT seem to be all and only the levels within \( S_{tot}^0 = 0 \), while those with \( S_{tot}^0 \neq 0 \) maintain a finite energy gap in the limit of large \( L \). Hence, the reference state for the calculation of \( v \) will be the second excited state in \( S_{tot}^0 = 0 \), corresponding to the primary field of conformal dimensions \( (1/2,1/2) \).

Using quadratic extrapolations in \( 1/L \) we get \( v = 2.44 \), and consequently \( e_\infty = -2.0011961 \pm 0.0000006 \) and \( c = 0.5008 \pm 0.0008 \), thereby confirming the Ising universality class. The scaling dimensions can be estimated from the slopes of the straight lines in a plot like that of Fig.4. In Table 1 the theoretical values anticipated in Sect.4 are compared with these numerical estimates. The overall agreement is good (7% in the worst case). Note that all the marginal operators have nonzero momentum and so they cannot represent a valid perturbation to the continuum Hamiltonian in as much as they would break translational invariance. The absence of marginal operators suggests that each point of the Haldane-Néel transition corresponds to the same \( c = 1/2 \) theory and the line in the phase diagram is "generated" by the mapping from the discrete spin model to the continuum CFT. Repeating the same passages at \( \lambda = 1 \) we get \( D_c(1) = -0.315 \), \( \nu(1) = 1.003 \pm 0.006 \) together with \( v = 2.65 \), \( e_\infty = -1.62651 \), \( c = 0.498 \pm 0.002 \), that is, again a \( c = 1/2 \) continuum theory.

We now pass to an example of numerical investigation of a \( c = 1 \) line of
Figure 4: Energy differences, divided by $2\pi$, plotted vs $1/L$ at the Ising transition ($\lambda = 0.5, D = -1.2$). Points represent the numerical values obtained with multi-target DMRG runs ($M = 216$) collecting nine excited states within $S^z_{\text{tot}} = 0$. Continuous lines are best-fit whose slopes are given in Table 1, together with the theoretical predictions of the scaling dimensions (the labels on the right indicate the multiplicities, all correctly met).

critical points, namely the transition from the Haldane to the large-$D$ phase. In the past [20], a similarity with the critical fan of the Ashkin-Teller model has been suggested. The operator content of this model arises from Ginsparg’s orbifold construction [24] and consists of a number of $K$-independent scaling dimensions plus the contributions coming from the pure Gaussian part (free boson) discussed in the previous Section. The fact that we do not observe $K$-independent dimensions (apart from trivial secondaries of the identity) indicates that the continuum description of our spin-1 Hamiltonian with $PBC$ at the Haldane-large-$D$ transition should be purely Gaussian rather than "orbifold-like".

In order to support this claim, we try again to match the whole spectrum of the relevant and marginal operators ($d \leq 2$). The difference with the $c = 1/2$ case is that here we have to fix not one but two nonuniversal parameters, $\nu$ and $K$ (see Eq. (50)). As regards the former, the velocity stems from the first and second excited states in $S^z_{\text{tot}} = 0$. Note that in choosing these levels we are assuming, self-consistently, that $K > 1$ so that the two secondaries of the identity ($d = 1$) come first than the primaries with $(m = 0, n = \pm 1)$, having $d_{0,\pm 1} = K$. As far as the Luttinger parameter $K$ is concerned, we have to inspect the spectrum in other sectors of $S^z_{\text{tot}}$ too. In particular, the first excited state lies in $|S^z_{\text{tot}}| = 1$, that corresponds to $m = \pm 1, n = 0$ in Eq. (50). The value of $K$ is obtained from the slope $d_{\pm 1,0} = 1/4K$ in a plot similar to that of Fig.4.
More generally, in order to check the self-consistency of the hypothesis \( c = 1 \), we have computed the finite-size spectrum of relevant and marginal operators in different sectors of \( S^2_{\text{tot}} \) for a couple of critical points on the Haldane-large-\( D \) line (first two rows of Table 2). Once that \( v \) and \( K \) are numerically determined, the structure of the Gaussian spectrum is correctly reproduced (including the multiplicities) and the overall comparison is satisfactory since, in worst cases, the relative difference does not exceed 3\% (see plots and tables of Ref. [17]).

Table 2: Velocity, central charge and ground state energy density for some critical points on the Haldane-large-\( D \) transition line. The numbers are the outcome of DMRG calculations with \( L = 16, 20, 24, 32, 48, 64 \) and \( M = 405 \), for cases with \( K > 1 \), or \( L = 16, 20, 24, 28, 32, 36, 40 \) and \( M = 400 \), for cases with \( K < 1 \). The last two columns contain the numerical estimate of the nonuniversal parameter \( K \), (according to the procedures described in the text) and the gap exponent obtained from the CFT formula \( \nu = 1/(2 - K) \). The error on \( \nu \) is typically of one unit in the last digit or better.

| \( [\lambda, D_c(\lambda)] \) | \( v \) | \( c \) | \( \epsilon_{\infty} \) | \( K \) | \( \nu \) |
|----------------|--------|--------|----------------|--------|--------|
| (0.50, 0.65) | 2.197 ± 0.004 | 1.008 ± 0.003 | −0.908765 | 1.580 ± 0.004 | 2.38 |
| (1.00, 0.99) | 2.588 ± 0.006 | 0.997 ± 0.003 | −0.859152 | 1.328 ± 0.004 | 1.49 |
| (2.59, 2.30) | 3.70 ± 0.04 | 0.99 ± 0.01 | −0.675099 | 0.85 ± 0.01 | 0.870 |
| (3.20, 2.90) | 4.445 ± 0.005 | 1.133 ± 0.006 | −0.59132 | 0.526 ± 0.007 | 0.678 |

Enforced by these quantitative predictions, we try to approach the multicritical point where the \( c = 1 \) line meets the \( c = 1/2 \) one. Supposedly, the central charge at this point is \( c = 3/2 \) and it has been proposed [49] that the corresponding CFT is a SU(2)$_2$ Wess-Zumino-Witten-Novikov model. If this was true, the two lines should join at the point where the effective Gaussian theory has \( K = 1 \) [27] (\( FD \) point). Using \( \lambda \simeq D \) in the expression of \( g \) we find that \( K = \pi/g(\lambda) = 1 \) is satisfied for \( \lambda \simeq 2 \), while it is believed [13] that the multicritical point lies at \( \lambda \gtrsim 3 \). We guess that the two lines join at \( K < 1 \), and in order to test this conjecture we study two more points: \((\lambda = 2.59, D = 2.30)\), again on the \( c = 1 \) line, and \((\lambda = 3.20, D = 2.90)\) proposed in [13] as the multicritical point itself. Although the steps are conceptually the same as above, here we encounter two additional complications. First, due to the closeness (or almost coincidence in the multicritical case) of the Ising transition, we observe the merging of the two (quasi)critical spectra. Hence, we have to target more states and separate the ones belonging to \( c = 1 \) from the ones belonging instead to \( c = 1/2 \). Second, we observe sizeable finite-size corrections from irrelevant operators. In fact, our analysis shows that we are moving at values of \( K \) smaller than one towards \( K = 1/2 \) where certain irrelevant operators become marginal. As explained in [17], the last two rows of Table 2 are obtained by extracting \( K \) not from the first excited state, but rather from half the sum of the pair of levels with \( m = 0, n = \pm 1 \) in \( S^2_{\text{tot}} = 0 \), to get rid of finite-size corrections.
keeps on decreasing towards 1/2 (SD point) where we argue that this line meets the Haldane-Néel one and a first order transition starts.

We close the section with a few comments on the hidden topological order measured by string order parameters (Eq. 23). It is expected that, leaving the Haldane phase, the \( Z_2 \times Z_2 \) symmetry is partially or totally restored. As customary, we can introduce two off-critical exponents that control the closure of these order parameters. For instance, fixing \( \lambda \) and varying \( D \) about \( D_c(\lambda) \):

\[
O^z_S \propto (D_c - D)^{2\beta^z_S}, \quad O^x_S \propto (D_c - D)^{2\beta^x_S}
\]

Now, according to FSS arguments (sec. 5.1 of [24]), \( \beta^z_S \) and \( \beta^x_S \) are related, via the gap exponent \( \nu \), to their counterparts at criticality, that is, the scaling dimensions of the operators entering the associated string correlation functions. These dimensions, in turn, can be extracted from the slopes, \( \eta_S \) and \( \eta^z_S \), in the log-log plots of \( O^{z \times z}_S (D = D_c) \) evaluated at half of the chain. Using the relation \( 2\beta^z_S = \nu \eta^z_S \) (and analogously for the \( z \) channel) we find the values reported in Table 3 for a couple of critical points already discussed above. We should observe that the scaling dimensions \( \eta_S/2 \) and \( \eta^z_S/2 \) are not contained in the \( c = 1 \) spectra cited above. However, we notice also that the numerical estimates of \( \eta^z_S \) are rather close to the values \( 2\beta^z_S = K/2 \) and that these levels actually exist in the effective continuum theory provided that half-integer values of \( n \) are allowed in Eq. (50). In the XXZ spin-1/2 formulation this is known to correspond to twisted boundary conditions on the chain. Thus, considering that the calculations presented here for the spin-1 case are with PBC, it’s not surprising that the scaling dimensions associated with \( O^{z \times z}_S \) are absent in the numerical spectra. Nonetheless, we believe that the closeness to \( K/2 \) is not accidental and in Ref. [17] we speculated about the possibility that the longitudinal string correlation functions (Eq. (21) with \( \alpha = z \) ) acquires, in the continuum limit, the asymptotic form

\[
G^z_S (r) \sim \langle \exp \left[ \mp i \pi K \Phi(0) \right] \exp \left[ \pm i \pi K \Phi(r) \right] \rangle
\]

so that the lattice string \( S^0 \) \( \exp \left[ i\pi \sum_{l=1}^{r-1} S_l^z \right] \) is somehow related to the continuum twist operator \( \exp \left[ \pm i \pi K \Phi(r) \right] \).

Table 3: Exponents associated with the vanishing string order parameters at the Gaussian transitions taking place at the points indicated in the first column (see text for definitions). All the numbers are obtained with FSS on the data at \( L = 32, 48, 64, 80, 100 \) and \( M = 300 \).

| \( \lambda, D_c(\lambda) \) | \( 2\beta^z_S \) | \( 2\beta^x_S \) | \( \eta_S \) | \( \eta^z_S \) |
|--------------------------|---------------|---------------|-----------|-----------|
| (0.50,0.65)              | 0.597 ± 0.009 | 1.91 ± 0.02   | 0.251 ± 0.002 | 0.804 ± 0.003 |
| (1.00,0.99)              | 0.407 ± 0.002 | 1.10 ± 0.01   | 0.273 ± 0.0006 | 0.741 ± 0.002 |

6 Conclusions.

In the present paper we have reviewed, to the best of our knowledge, part of the status-of-the-art concerning Heisenberg spin chains, including biquadratic
interaction terms and various kinds of anisotropies, concentrating on the role of hidden symmetries in the various families of spin models. We have discussed how the inclusion of anisotropy terms can drive the "standard" Heisenberg chain away from the Haldane phase and how hidden symmetries (and their spontaneous breaking) are of great help in classifying the "massive" (gapful) phases of the model. The location of the critical lines of the model has been accurately obtained numerically, confirming and extending earlier predictions [13].

The combined use proposed here of analytical (CFT) and numerical (DMRG) techniques to investigate the critical properties of the models has proved to be a rather successful strategy to clarify the nature and structure of the critical phases of the models. Numerical simulation techniques (Monte Carlo and DMRG, to quote only the most known ones) are of more and more frequent and extended use in almost all branches of Theoretical Physics. A blind use of them can however be more dangerous than helpful in understanding the physical properties of the systems for whose study they are employed. We believe instead that an "educated" use of numerical techniques in support of analytical approaches, as described here, can result in a powerful synergy that can be of great help in understanding the physics of many problems in Theoretical Physics.

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