Chiral order in spin-S XY chains

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We consider the issue of chiral ordering in spin chains for an arbitrary value of the spins \( S \). By use of bosonization according to a scheme developped by H.-J. Schulz, we obtain the phase diagram of the chain with XY exchange couplings between nearest and next-to-nearest neighbors. We obtain a satisfactory picture including a so-called chiral spin nematic phase which is gapless, has long-range chiral order and incommensurate spin correlations. We perform a stability analysis of this phase and point out that this analysis is in conflict with existing DMRG results that shows a difference between integer and half-integer spin case.

§1. Introduction

Quantum antiferromagnetic spin chains display a variety of phases that have no classical counterpart. This variety is even increased if we consider the effect of frustration. Many studies\textsuperscript{1) have been devoted in the past to the simple AF chain with nearest neighbor exchange \( J_1 \) and next-to-nearest neighbor \( J_2 \). In the isotropic case, the Hamiltonian is then simply:

\begin{equation}
\mathcal{H} = J_1 \sum_n (S_n S_{n+1}) + J_2 \sum_n (S_n S_{n+2}),
\end{equation}

where \( S_n^+ = S_n^x \pm iS_n^y \) is a spin operator at site \( n \) and there are competing antiferromagnetic interactions \( J_1, J_2 > 0 \) which introduces frustration in the model. In the spin-1/2 case, for small \( J_2 \), there is a spin-fluid phase whose effective theory is that of a massless free boson. It has quasi-long range spin order with algebraic decay of spin correlations. For larger values of \( J_2 \), the ground state is spontaneously dimerized : this appears through a quantum phase transition of Kosterlitz-Thouless type.

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and eventually incommensurability develops within this gapped phase for even larger values of $J_2$ but without any additional phase transition. The situation is remarkably different if we now consider XY exchange:

$$
\mathcal{H} = J_1 \sum_n (S^x_n S^x_{n+1} + S^y_n S^y_{n+1}) + J_2 \sum_n (S^x_n S^x_{n+2} + S^y_n S^y_{n+2}).
$$  \hspace{1cm} (1.2)

Starting from the limit with large $J_2$, Nersesyan et al.\cite{2} used a mean-field treatment and then bosonization to predict the occurrence of a new phase with many unconventional characteristics. In this limit, they predicted that there is long-range chiral order:

$$
\langle (\vec{S}_n \wedge \vec{S}_{n+1})_z \rangle \neq 0.
$$  \hspace{1cm} (1.3)

There are also local spin currents polarized along the anisotropy $z$-axis. This phase is gapless and there are incommensurate spin correlations that decay algebraically with an exponent which they found to be $1/4$. The existence of this phase has been recently demonstrated numerically. Such a phase has been disclosed in a ladder model formulated first as an array of Josephson junctions which is equivalent to a spin-1/2 half model\cite{3}. this ladder has square plaquettes so it is not frustrated as model Eq.(1.2) but frustration is introduced by half a flux quantum piercing the plaquettes. Then a study\cite{4} using the DMRG algorithm gave evidence for this phase in model Eq.(1.2) : the spin fluid phase is stable up to $J_1/J_2 \approx 0.33$ then the chain undergoes dimerization and at $J_1/J_2 \approx 1.26$ there is a second transition to the chiral critical phase. This new phase has also been reported\cite{5,6} in the S=1 chain with the same Hamiltonian Eq.(1.2). Here the situation is even more richer. When $J_2 = 0$, we are in the XY phase which destroyed immediately by adding even an infinitesimal $J_2$, the phase that appears then is the celebrated gapped Haldane phase. This phase resists the perturbing influence of $J_2$ for a while but at $J_1/J_2 \approx 0.47$ there is a phase transition to chiral order but the gap remains nonzero. Then very close, at $J_1/J_2 \approx 0.49$, there is a distinct transition to a critical phase with chiral order as in the S=1/2 case. So the integer S=1 case has an additional phase w.r.t. the S=1/2 case, a gapped chiral phase. This difference persists for higher spins\cite{7}. For S=3/2, there is an intermediate dimerized phase which is replaced in a single transition by a chiral critical phase. For S=2, the Haldane phase is destroyed by two successive transitions as for S=1. To understand this pattern of phase transition we use the bosonization technique which has been adapted to the case of generic spin-S by Schulz\cite{8}. This method is able to capture the phase diagrams as a function of exchange anisotropy as well as single-ion anisotropy and it correctly captures the
§ 2. Weak coupling limit

The idea is to write down each spin-S as a sum spins 1/2:

$$S^+_n = \sum_{a=1}^{2S} \lambda_{a,n}^+.$$  

Each spin 1/2 is then bosonized by the standard technique. There is a bosonic field $\phi_a, a = 1 \ldots 2S$ associated with each spin. The first possibility is to treat $J_2$ as a perturbation. So we start from an isolated spin-S chain and write its effective theory in terms of the bosons $\phi_a$. Due to the appearance of couplings $s^+_a s^-_b$, there are operators that induce gaps for some linear combination of the basic bose field. More precisely, only the "acoustic" mode remains massless:

$$\Phi = \frac{1}{\sqrt{2S}} (\phi_1 + \ldots + \phi_{2S}).$$

The effective Hamiltonian for the acoustic mode is thus a simple free theory:

$$H_{XY1} \simeq \frac{v}{2} \left( \Pi^2 + (\partial_x \Phi)^2 \right),$$

where $\Pi$ is the canonical momentum conjugate to $\Phi$. The coefficient $v$ is an unimportant velocity and we have used the conventional name "XY1" coming from the standard S=1 chain phase diagram. The spin operator can be expressed in terms of the field $\Theta$ which is dual to $\Phi$:

$$S^\pm \sim (-1)^{\mp a} \exp \left( \pm i \sqrt{\pi/2S} \Theta \right).$$

This expression shows easily that the XY spin correlations decay algebraically with an exponent $\eta = 1/4S$. This is in agreement with numerical findings \cite{10}. In the S=1 case it is also in agreement with work by Kitazawa et al. \cite{11}. If we now bosonize the perturbation $J_2$, we find that there is a simple renormalization of the previous free hamiltonian Eq.(2.3) but in addition vertex operators appear in perturbation expansion. For integer spin, the most relevant operator appear at $S^{th}$ order and it appears at $2S^{th}$ order for half-integer spins. The effective theory is then:

$$H \simeq \frac{v}{2} \left( K \Pi^2 + \frac{1}{K} (\partial_x \Phi)^2 \right) - \frac{g_{eff}}{a} \cos(\beta \Phi),$$

where $\beta = \sqrt{8\pi S}$ for integer spins and $\beta = \sqrt{32\pi S}$ for half-integer spins. The Luttinger parameter $K$ is obtained in perturbation $K = 1 - (4/\pi)J_2/J_1 + O(J_2^2)$. 

The difference between integer and half-integer spins.
This effective leads then immediately to the phase diagram of the spin-$S$ XY chain for small $J_2/J_1$. The scaling dimension of the vertex operator in the effective theory Eq. (2,3) is \( K \beta^2/4\pi \) and thus is irrelevant for small $J_2$, the XY1 phase will have thus a finite extent. With increasing $J_2$, the vertex operator becomes relevant and drives the system towards a massive phase through a KT transition. Depending upon the spin parity, it will be the Haldane or the dimerized phase. If we take seriously the approximate formula for $K$, we deduce $J_2/J_1 \approx 0.29$ at the KT transition for $S=1/2$, which compares quite favorably to the numerical estimate of $\approx 0.324$. We also predict that $S=1$ is special: in this case indeed the operator is marginal for $J_2 \to 0$ hence the instability takes place immediately upon switching an infinitesimal value of $J_2$, as seen in DMRG studies.

§3. Zigzag limit

We now turn to the opposite limit $J_2 \gg J_1$. Then we have a two-leg spin-$S$ XY ladder coupled in a zigzag way. We first bosonize the two independent legs when $J_1 = 0$. So each of the chains can be treated as in the previous section. There are now two acoustic modes $\Phi_1$ and $\Phi_2$ that are the effective low-energy degrees of freedom. It is convenient to introduce the symmetric and antisymmetric combinations of these two modes:

\[
\Phi_\pm = \frac{1}{\sqrt{2}} (\Phi_1 \pm \Phi_2).
\]

(3.1)

The leading contribution to spin correlations comes from the following operator:

\[
S_\pm^a \simeq \frac{\lambda}{\sqrt{a}} (-1)^{x/a} \exp \left( \mp i \sqrt{\pi/2S} \Theta_\pm \right),
\]

(3.2)

where $a = 1, 2$ and $\Theta_\pm$ are the fields dual to $\Phi_\pm$. When $J_1 = 0$ the two fields $\Phi_\pm$ are free and massless. Introducing $J_1$, we find the effective theory:

\[
\mathcal{H} \simeq \frac{v}{2} \sum_{a=\pm} \left( \Pi_\pm^2 + (\partial_x \Phi_\pm)^2 \right) + g \partial_x \Theta_+ \sin \left( \sqrt{\frac{\pi}{2S}} \Theta_- \right),
\]

(3.3)

where $\Theta_\pm$ are fields dual to $\Phi_\pm$ and $\Pi_\pm$ are canonical conjugate to $\Phi_\pm$, and $g = O(J_1)$. The operator perturbing the free part in Eq. (3.3) is a parity symmetry breaking term with nonzero conformal spin ($=1$). Its effect is thus highly nontrivial. A simple perturbation with nonzero conformal spin is given by the uniform component of the spin density $\partial_x \Phi$. In this case we know its effect: it induces incommensurability.

We treat theory Eq. (3.3) by following exactly the method of nersesyan et al. We
just decouple:
\[ \partial_x \Theta_+ \sin \left( \sqrt{\frac{\pi}{S}} \Theta_- \right) \rightarrow \kappa < \partial_x \Theta_+ > + \mu < \sin \left( \sqrt{\frac{\pi}{S}} \Theta_- \right) >. \] (3.4)

We then impose self-consistency. The "+" sector remains massless while the "-" sector is massive due to the vertex operator in Eq.(3.4). The results that follow are then close to the original findings for for S=1/2 critical chiral phase. The most notable difference is that spin correlations decay algebraically with a spin-dependent exponent:
\[ \langle S^1_+ (x) S^a_- (0) \rangle \sim \frac{e^{iqx}}{|x|^{1/(8S)}}, \quad a = 1, 2, \] (3.5)

with \( q - \pi/a \sim (J_1/J_2)^{4S/(4S-1)} \). The exponent 1/4 of the S=1/2 case is thus a special case of \( \eta = 1/8S \). This formula is in good agreement with measurements by DMRG up to S=2. There are nontrivial spin currents in the ground state:
\[ \langle J^1_z \rangle = \langle J^2_z \rangle = -v \sqrt{\frac{S}{\pi}} \langle \partial_x \Theta_+ \rangle \neq 0. \] (3.6)

In the language of spins, this means intrachain currents:
\[ \langle (\vec{S}_{a,n} \wedge \vec{S}_{a,n+1})_z \rangle \propto \sqrt{\frac{\pi}{4S}} \langle \partial_x \Theta_+ \rangle \neq 0, \quad a = 1, 2, \] (3.7)
as well as interchain currents:
\[ J_1 \langle (\vec{S}_{1,n} \wedge \vec{S}_{2,n})_z \rangle \propto \langle \sin \left( \sqrt{\frac{\pi}{S}} \Theta_- \right) \rangle \neq 0, \] (3.8)

this also means long-range chiral order.

§4. Stability analysis

We certainly expect that when increasing the coupling \( J_1 \) the "+" sector of theory (3.3) will not remain massless forever because we know from the analysis of the previous approach in the small \( J_2 \) limit that there is a massive phase. It is likely that some vertex operator will become relevant at some finite value of \( J_1/J_2 \). We try to find this operator by analyzing the symmetry properties of the theory. Taking into account the symmetries of the mean-field Hamiltonian, we find the following effective theory:
\[ \mathcal{H}_+ \simeq \frac{v}{2} \left( K \Pi^2_+ + \frac{1}{K} (\partial_x \Phi_+)^2 \right) + \kappa \partial_x \Theta_+ - \frac{g_{eff}}{a} \cos (\gamma \Phi_+), \] (4.1)

where \( \gamma = \sqrt{16\pi S} \) for integer S and \( \gamma = \sqrt{64\pi S} \) for half-integer spins. When this vertex operator becomes relevant, the system is gapped and still incommensurate.
This is consistent with the observation of a "chiral Haldane" phase in numerical studies for integer spins. For half-integer spin, this predicts a phase which is dimerized (due to the value at which $\Phi$ is pinned) and has chiral LRO. We are then forced to speculate that there is then an additional Ising transition at which chiral LRO disappear to make contact with the small $J_2$ limit.

§5. Conclusions

The bosonization approach is able to reproduce the phase diagram of the XY $J_1 - J_2$ chain for integer spins. For all spins it correctly predicts the existence of the chiral critical phase. The spin correlations decay with exponent $1/8S$. For the half-integer case, this approach predicts a dimerized phase with incommensurability and chiral order which is apparently not seen. It is possible that this signals a failure of the mean-field decoupling. For integer spins, there is good agreement with a large-S study\cite{12}. A possible candidate\cite{13} for the chiral critical phase for $S=1$ is CaV$_2$O$_4$ which has $J_1 \approx J_2$. This would require a large single-ion anisotropy\cite{14} to escape from the double Haldane phase.

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