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Nonlinear sigma model study of a frustrated spin ladder

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Abstract. A model of a two-leg spin-*S* ladder with two additional frustrating diagonal exchange couplings J_D , J'_D is studied within the framework of the nonlinear sigma model approach. The phase diagram has a rich structure and contains 2*S* gapless phase boundaries which split off the boundary to the fully saturated ferromagnetic phase when J_D and J'_D become different. For the S = 1/2 case, the phase boundary is identified as separating two topologically distinct Haldane-type phases as discussed recently by Kim and co-workers (Kim E H, Fáth G, Sólyom J and Scalapino D J 1999 *e-print* cond-mat/9910023).

1. Introduction

Low-dimensional spin models still continue to attract a considerable amount of attention from researchers, both as regards theoretical and experimental aspects. Since the famous prediction of Haldane in 1983 [1] of different behaviours of Heisenberg spin chains with integer and half-integer values of the spin *S*, which was based on a mapping to the nonlinear sigma model (NLSM), the NLSM approach has been recognized as an important tool in studying spin systems and has found numerous applications (see, e.g., [2] for a review). Normally, the NLSM approach does not give good numerical results; however, it is usually able to capture the topology of the phase diagram.

During the recent upsurge of interest in spin-ladder models, several researchers have successfully applied the NLSM to describe an *N*-leg spin-*S* ladder [3–5]. An essential similarity to the case of a single chain was found: for half-integer *S*, the ladders with even or odd numbers of legs *N* are respectively gapped and gapless. A natural question arose, namely, that of whether the properties of a gapped phase of, say, a two-leg spin- $\frac{1}{2}$ ladder are in some sense equivalent to those of the Haldane phase of a spin-1 chain.

Several arguments were given in favour of the positive answer to the above question [6–8]. In particular, it was shown that by adding extra interactions one can introduce a suitable generalization of the pure ladder model, increasing the number of parameters in the phase space, and then one can find a path in this generalized phase space which smoothly (i.e., without crossing any phase boundaries) leads from the ladder model to a certain composite representation of a spin-1 chain [6, 8]; moreover, it was demonstrated [6, 7] that a two-leg $S = \frac{1}{2}$ ladder has nonzero string order which is believed [9] to be a characteristic feature of the Haldane phase.

On the other hand, it turned out that other generalizations may have very different properties; for instance, for the model of a 'diagonal ladder' with additional equal-strength 960 *C-M Nedelcu et al*

diagonal interactions, which also yields a composite-spin representation of a spin-1 chain [10], one finds numerically that the 'usual' ladder is separated from the composite-spin-1 Haldane phase by a transition line [11, 12]. An exactly solvable model exhibiting similar features was also constructed [13].

Recently, Kim *et al* [14] have made an interesting observation, noticing that there are actually at least *two* different definitions of the string order for a two-leg spin- $\frac{1}{2}$ ladder (depending on whether one combines the $S = \frac{1}{2}$ spins on the rungs or on the diagonals). Exploiting the analogy with the topological quantum numbers which can be introduced for short-range valence bond states on a square lattice [15], they have conjectured that those two definitions of the string order distinguish between *two different Haldane-type phases*. This assumption was supported by the results of the bosonization study of two generalizations of the ladder model.

In the hope of getting a better understanding of the physics of the spin ladder, and to search for possible new phase transitions, we find it interesting to study the phase diagram of the generalized ladder model with unequal diagonal couplings. We consider the model determined by the Hamiltonian

$$\widehat{H} = J_L \sum_{\alpha=1,2} \sum_i S_{\alpha,i} \cdot S_{\alpha,i+1} + J_R \sum_i S_{1,i} \cdot S_{2,i} + \sum_i (J_D S_{1,i} \cdot S_{2,i+1} + J'_D S_{2,i} \cdot S_{1,i+1})$$
(1)

where $S_{\alpha,i}$ are spin-S operators at the *i*th rung; $\alpha = 1, 2$ distinguishes the ladder legs. The model is shown schematically in figure 1. At $J_D = J'_D = 0$ one recovers a regular ladder, while at $J'_D = 0$ the model is equivalent to a zigzag chain with alternation of the nearest-neighbour interaction. Interchanging J_D and J'_D is obviously equivalent to interchanging the legs of the ladder, so it is sufficient to restrict ourselves to the $J_D \ge J'_D$ case. The point $J_D = J'_D$ is in a certain sense special, since it allows an additional symmetry operation—that is, interchanging the spins on every other rung is then equivalent to interchanging J_D and J'_L .





The phase space of the model is three dimensional and is determined by the three ratios of exchange constants, e.g., J_D/J_R , J'_D/J_R , J_L/J_R . We will show that for $J_D \neq J'_D$ the phase diagram of the above model always possesses 2*S* gapless phase planes, which split off the boundary to the fully saturated ferromagnetic phase at $J_D = J'_D$. We consider in detail the most interesting case $S = \frac{1}{2}$ and show that the gapless plane is an extension of one of the transition lines discussed in reference [14]. In the next section we briefly describe the mapping to the NLSM, section 3 contains the discussion of the results, and, finally, section 4 gives a brief summary.

2. Results of the mapping to the nonlinear sigma model

To map the model (1) to a NLSM, we use the well-known technique of the spin-coherentstates path integral; this technique is well described in reviews and textbooks [2], and here we will not give a complete derivation but rather indicate just the main steps. We choose a four-spin plaquette as an elementary magnetic cell; then there are four classical ground states *commensurate* with this choice of cell, namely a ferromagnetic state (F) and three modulated states shown in figure 1 and denoted as A, B and C. At the *n*th plaquette we introduce four variables m_n , l_n , u_n , v_n , defined as the following linear combinations of the 'classical' spin vectors (parameters of the coherent states):

$$l_{n} = \frac{1}{4S} (S_{1,2n-1} + S_{2,2n-1} - S_{1,2n} - S_{2,2n})$$

$$m_{n} = \frac{1}{4S} (S_{1,2n-1} + S_{2,2n-1} + S_{1,2n} + S_{2,2n})$$

$$u_{n} = \frac{1}{4S} (S_{1,2n} + S_{2,2n-1} - S_{1,2n-1} - S_{2,2n})$$

$$v_{n} = \frac{1}{4S} (S_{2,2n-1} + S_{2,2n} - S_{1,2n-1} - S_{1,2n})$$
(2)

which satisfy the following four constraints:

$$m^{2} + l^{2} + u^{2} + v^{2} = 1$$

$$(m + l) \cdot (u + v) = 0$$

$$(m - l) \cdot (u - v) = 0$$

$$(m + v) \cdot (u + l) = 0.$$
(3)

These variables we consider as smoothly varying functions of the space coordinate $x_n = na$ when passing to the continuum limit; one should mention that the above *ansatz* is essentially similar to that used by Sénéchal [4]. The advantage of the *ansatz* (2) is that it conserves the total number of degrees of freedom, which is important for avoiding ambiguities in the mapping, as was recently realized for the example of inhomogeneous spin chains [16].

The order parameters for the four commensurate classical ground-state configurations F, A, B, C are respectively m, u, v, l. Comparing the energies of those configurations, one may obtain a 'draft' of the classical phase diagram which neglects the presence of any incommensurate ground states; for the moment we are mainly interested in the commensurate antiferromagnetic part, and the conditions for the existence of spiral phases will be obtained later. One thus may treat m as a small fluctuation, and obtain different field descriptions starting from one of the configurations A, B, C. Massive degrees of freedom can be integrated out in a usual way, and in each case one obtains the final effective action in the form of a NLSM:

$$\mathcal{A}_{\rm eff}/\hbar = \frac{1}{2g} \int \int d\xi \, d\tau \, \{(\partial_{\tau} n)^2 - (\partial_{\xi} n)^2\} + \frac{\theta}{4\pi} \int \int d\xi \, d\tau \, n \cdot (\partial_{\xi} n \times \partial_{\tau} n) \tag{4}$$

where *n* is the corresponding order parameter, and $\xi = x/a$, $\tau = ct/a$ are dimensionless space-time variables, *a* being the lattice constant along the leg direction. For each of the classical 'phases' A, B, C the coupling constant *g* and the topological angle θ are given by the following expressions:

Phase A: $J_R + 2J_L > 0$, $J_D^+ < J_R$, $J_D^+ < 2J_L$:

$$g_{A} = \frac{J_{R} + 2J_{L}}{2S\sqrt{W_{A}}} \qquad \theta_{A} = 0 \mod 2\pi$$

$$W_{A} = \frac{1}{4}(J_{R} + 2J_{L}) \left\{ 2J_{L} - J_{D}^{+} - \frac{(J_{D}^{-})^{2}}{J_{R} - J_{D}^{+}} \right\} > 0.$$
(5)

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Phase B: $J_R + J_D^+ > 0$, $2J_L < J_D^+$, $2J_L < J_R$:

$$g_B = \frac{J_R + J_D^+}{2S\sqrt{W_B}} \qquad \theta_B = \frac{4\pi SJ_D^-}{J_R + J_D^+} W_B = \frac{1}{4} \{ (J_R + J_D^+) (J_D^+ - 2J_L) - (J_D^-)^2 \} > 0.$$
(6)

Phase C: $J_D^+ + 2J_L > 0$, $J_R < J_D^+$, $J_R < 2J_L$:

$$g_{C} = \frac{J_{D}^{+} + 2J_{L}}{2S\sqrt{W_{C}}} \qquad \theta_{C} = 0 \mod 2\pi$$

$$W_{C} = \frac{1}{4}(J_{D}^{+} + 2J_{L}) \left\{ 2J_{L} + J_{D}^{+} - \frac{(J_{D}^{-})^{2}}{J_{D}^{+} - J_{R}} \right\} > 0.$$
(7)

Here for the sake of convenience we have introduced the notation

$$J_D^{\pm} \equiv (J_D \pm J_D').$$

The spin-wave velocity for each case is given by $c = 2\sqrt{W}Sa/\hbar$. The inequalities define the boundaries of the domains of validity of the corresponding mapping (not all of them represent real phase boundaries, as will be discussed later). The boundaries defined by $W_{A,B,C} = 0$ represent just the classical conditions for the transition into a spiral phase. One may observe that there is no spiral phase at $J_D^- = 0$.

Phase F has to be considered separately, and it is easy to obtain its boundaries using the linear spin-wave theory. There are two magnon branches with the energies

$$\varepsilon_{\pm}(q) = -S(J_R + J_D^+ + 2J_L) + 2SJ_L \cos q \pm S\{(J_R + J_D^+ \cos q)^2 + (J_D^- \sin q)^2\}^{1/2}$$
(8)

and from the condition of positiveness of ε_{\pm} it is easy to obtain the boundaries of the F phase. They are determined by the inequalities

$$J_R + J_D^+ > 0 \qquad J_R + 2J_L > 0 W_F \equiv -2J_L - J_D^+ + (J_D^-)^2 / (J_R + J_D^+) > 0.$$
(9)

At $W_F = 0$, $\varepsilon_-(q)$ changes sign at once in a finite interval of wave vectors near q = 0, signalling the first-order transition, $\varepsilon_-(q = \pi)$ vanishes at the line $J_R + 2J_L = 0$, and $\varepsilon_+(q = 0)$ becomes zero at the line $J_R + J_D^+ = 0$.

One can see that only in the B case is there a nontrivial topological term, and the condition of gaplessness $\theta = (2n + 1)\pi$ yields

$$J_D^- = \frac{2n+1}{4S}(J_R + J_D^+) \qquad n = 0, 1, \dots, 2S - 1.$$
(10)

One can see that the 2S gapless planes (10) exist only at nonzero J_D^- , and at $J_D^- = 0$ they split off the boundary $J_R + J_D^+ = 0$ to the ferromagnetic phase.

3. Discussion

Let us concentrate on the case $S = \frac{1}{2}$ as being the most important one. For $S = \frac{1}{2}$, a sketch of the resulting phase diagram is presented in figure 2 in the form of two-dimensional slices through the phase space at three fixed values of J_D^- (J_R is considered to be positive).

At $J_D^- = 0$ there are no other gapless lines except the boundaries of the ferromagnetic phase, and there is no spiral phase. The coupling constants g_A , g_B diverge at the AB boundary $J_D^+ = 2J_L$, which indicates that this classical phase boundary gets destroyed by quantum fluctuations. On the other hand, all the coupling constants remain finite at the BC and AC

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Figure 2. A sketch of the phase diagram of the model (1); shown are the slices in the threedimensional phase space at fixed $J_D^- \equiv J_D - J'_D$: (a) $J_D^- = 0$; (b) $J_D^- = J_R$; (c) $J_D^- = 3J_R/2$. Thick solid and dashed lines denote the second- and first-order transition boundaries, respectively. Thin dashed lines indicate crossovers between different classical configurations; the coupling constant diverges at those lines. A, B, C are classical configurations shown in figure 1, F denotes the fully saturated ferromagnetic phase, and S stands for the spiral 'phase' inside which our approach is not valid. H1 and H2 denote topologically different Haldane-type phases with $\mathcal{O}_{even} \neq 0$ and $\mathcal{O}_{odd} \neq 0$ according to the classification of reference [14].

boundaries, but they undergo a jump when crossing the boundaries, which suggests a first-order transition. This is in agreement with the numerical [11, 12] and bosonization [11, 14] studies, showing the presence of a first-order transition with $J_D = J_R/2$ being the asymptote for the transition line at $J_L \rightarrow \infty$. There is also a 'mirror' transition line $J_L = J_R/2$ due to the $J_D \leftrightarrow J_L$ symmetry. According to the classification of reference [14], these two first-order transition lines separate two topologically different Haldane-type phases with $\mathcal{O}_{\text{even}} \neq 0$ (phases A, B) and $\mathcal{O}_{\text{odd}} \neq 0$ (phase C); below, we refer to these two phases as H1 and H2 (see figure 2(a)).

At finite J_D^- , the spiral phase (S) appears classically in a finite region of the phase diagram. The S region is for us just a 'white spot' which cannot be treated within the present approach; to construct an effective description for the S phase, one has to employ different techniques. At finite J_D^- the gapless line $J_D^+ = 2J_D^- - J_R$ starts to split off the BF boundary $J_D^+ = J_R$, and the FS boundary becomes first order, as one sees from the behaviour of $\varepsilon_-(q)$ (cf. (8)). The

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coupling constants $g_{A,B,C}$ diverge at the boundaries to the S phase, which suggests destruction of any (quasi-) long-range order, and thus one may expect the gapless line to terminate at the BS boundary, though it may in principle continue as a first-order transition line.

It is worthwhile to look at the particular case $J_D^- = J_R$. According to reference [14], the gapless line $J_D^+ = J_R$ in this case also separates two phases with different string order, which implies that the lower portion of the B phase belongs to the H2 class. It is also known that in this case the gapless line continues at larger J_L as the first-order line (recall that $J_D^- = J_D^+ = J_R$ corresponds to the uniform spin chain with next-nearest-neighbour interaction). Thus, it becomes clear that additional phase boundaries should exist somewhere inside the spiral 'phase', to achieve a proper separation of H1- and H2-type phases (see figures 2(b), 2(c)). This could be an interesting topic for future work.

4. Summary

We have studied the phase diagram of the generalized ladder model with unequal diagonal couplings J_D , J'_D within the framework of the nonlinear sigma model. We show that the phase diagram has a rich structure including several first- and second-order transition boundaries. There exist 2S gapless phase boundaries which split off the boundary to the ferromagnetic phase at $J_D \neq J'_D$. We consider the case $S = \frac{1}{2}$ in more detail and show that the gapless plane is an extension of one of the transition lines discussed in reference [14] which separate Haldane-type phases with different topological order parameter. Still, several features of the phase diagram remain unclear and require further study.

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