

# Generalized nonlinear sigma model approach to alternating spin chains and ladders

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Received 6 September 1999

**Abstract.** We generalize the nonlinear sigma model treatment of quantum spin chains to cases including ferromagnetic bonds. When these bonds are strong enough, the classical ground state is no longer the standard Néel order and we present an extension of the known formalism to deal with this situation. We study the alternating ferromagnetic-antiferromagnetic spin chain introduced by Hida. The smooth crossover between decoupled dimers and the Haldane phase is semi-quantitatively reproduced. We study also a spin ladder with diagonal exchange couplings that interpolates between the gapped phase of the two-leg spin ladder and the Haldane phase. Here again we show that there is a good agreement between DMRG data and our analytical results.

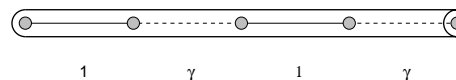
**PACS.** 75.10.Jm Quantized spin models – 75.20.Hr Local moment in compounds and alloys; Kondo effect, valence fluctuations, heavy fermions

## 1 Introduction

One-dimensional quantum spin systems exhibit remarkable physical properties. One of the most interesting case is the  $s = 1$  antiferromagnetic Heisenberg spin chain. Contrary to the  $s = 1/2$  case, this system has a gap as predicted by Haldane [1] and a finite spin correlation length. It is an example of a system which is disordered at zero temperature due to quantum fluctuations. The original conjecture has been checked experimentally [2], numerically [3] as well as analytically [4–6]. Although the ground state is disordered in the sense that spin correlations decay exponentially, there is a hidden topological order [7, 8] that is revealed in the bulk of the chain only by nonlocal observables or by ground state degeneracy in an open geometry. This hidden order is most clearly seen in the VBS wave function which is an approximate ground state of the spin-1 chain [5]. To construct this wave function one has first to write each spin  $s = 1$  as a triplet of two fictitious spins  $s = 1/2$ . Then one couples nearest-neighbor spins  $s = 1/2$  into singlets. This leads to a function which is obviously singlet and translation invariant. It is an excellent approximation of the true ground state [9]. The perfect crystalline pattern of singlets is the hidden order. Hida has given an appealing picture of the Haldane gap and the VBS ground state by considering an alternating ferro-antiferromagnetic  $s = 1/2$  chain [10]. The Hamiltonian is given by (see Fig. 1):

$$\mathcal{H} = J_{AF} \sum_n \mathbf{S}_{2n} \cdot \mathbf{S}_{2n+1} + J_F \sum_n \mathbf{S}_{2n+1} \cdot \mathbf{S}_{2n+2}. \quad (1.1)$$

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**Fig. 1.** The alternating ferro-antiferromagnetic spin chain. The coupling  $\gamma$  is the strength of the ferromagnetic bonds. The unit cell needed to construct a NL $\sigma$ M contains four spins.

Here  $\mathbf{S}_i$  are  $s = 1/2$  spin operators,  $J_{AF}$  is *positive* and  $J_F$  is *negative*. In what follows, we set  $J_{AF} = 1$  and  $J_F = -\gamma$ . The family of systems defined by equation (1.1) has simple limiting cases. For  $\gamma = 0$  we have a set of decoupled pairs of spins that have a trivial ground state: all pairs are locked in singlets. When  $\gamma \rightarrow \infty$ , the  $s = 1/2$  are coupled by pairs into  $s = 1$  states and we get a chain of spins  $s = 1$ . Hida has studied numerically the gap of the system as a function of  $\gamma$ . He has used Lanczos diagonalization techniques to evaluate the gap and he showed that there is no phase transition as a function of  $\gamma$ . As a consequence, the Haldane gap of the limit  $\gamma \rightarrow \infty$  is continuously connected to the trivial gap of the decoupled limit  $\gamma = 0$ . The excitation spectrum also evolves smoothly. So the alternating chain offers a simple physical picture of both the Haldane gap and the hidden topological order.

There is another approach to quantum spin chains which is the continuum field theory known as the nonlinear  $\sigma$  model (NL $\sigma$ M). Introduced originally by Haldane [1], this field theory includes a topological term [11]  $\theta = 2\pi s$  for a spin- $s$  chain. While this term can be discarded when  $s$  is integer, it is responsible for masslessness when  $\theta = \pi \pmod{2\pi}$ , *i.e.* for half-integer spin chain. This approach has been recently applied [12–14] to spin ladders where there is also a parity effect which is given by the number of legs of the ladder. Indeed, spin ladders with even

number of legs are generically gapped while odd-numbered ones are gapless. This effect can be explained in the NL $\sigma$ M framework with a topological term which is  $\theta = 2\pi s \times n_1$  where  $n_1$  is the number of legs. It is also of great interest to consider generalized spin ladders with various types of bond alternation and/or additional exchange couplings. For example, a spin ladder with a diagonal coupling interpolates smoothly [15] between the  $s = 1$  chain and the two-leg spin ladder. Previous investigations [16–21] of these more general situations have used the NL $\sigma$ M but with the impossibility to treat cases including ferro bonds as in the ferro-antiferro chain introduced by Hida.

In this work, we present a generalized NL $\sigma$ M that includes additional massive modes and we show that this model is able to reproduce the  $s = 1$  limit of alternating chain of Hida. We discuss the construction of this new effective theory in the path-integral framework although it could also be done in the Hamiltonian formalism with identical results.

In Section 2 we treat the alternating ferro-antiferromagnetic spin chain. From the spin-wave spectrum, we motivate the NL $\sigma$ M approach and obtain an approximate spin gap formula for the whole range of  $\gamma$ . In Section 3, we apply the same formalism to White's mapping from the spin-1 chain to the antiferromagnetic two-leg ladder. Section 4 contains our conclusions.

## 2 The alternating ferro-antiferromagnetic spin chain

### 2.1 Build-up of an effective sigma model

A NL $\sigma$ M for a spin chain is a non perturbative field theory which is built on the lowest energy modes of the classical theory of the chain. For the alternating chain equation (1.1) the dispersion relation of the spin waves is given by:

$$\omega(k) = s\sqrt{2\gamma(1+\gamma) \pm 2\gamma\sqrt{(1+\gamma)^2 - \sin^2 k}}. \quad (2.1)$$

The two lowest positive excitations correspond to momenta  $k_c = 0$  and  $k_c = \pi$ . Linearizing the dispersion relation around  $k_c$ , we obtain for those modes the linear relation  $\omega = s\sqrt{\frac{\gamma}{1+\gamma}}|k - k_c|$ . Hence the velocity of those spin waves is  $v = s\sqrt{\gamma/(1+\gamma)}$ . They stand for the two Goldstone modes of the (classically) broken  $O(3)$  symmetry. We will ground our NL $\sigma$ M on them, assuming they are slowly varying modes, in a theory where the rotational symmetry is unbroken. We also reasonably assume that the massive modes do not interfere significantly with the Goldstone modes, their energy being of the order of  $2s\sqrt{\gamma(1+\gamma)}$ .

Hida devised his alternating chain because of its appealing limit when the ferromagnetic exchange is getting to infinity. The limiting chain is an antiferromagnetic spin-1 chain with coupling  $J_{AF}/4$ . In this limit the ferromagnetic pairs are in a triplet state. Because of rotation invariance, the limiting Hamiltonian can be written as an

effective spin-1 chain. The couplings can only be quadratic  $\mathbf{S}_i \cdot \mathbf{S}_j$  or quartic  $(\mathbf{S}_i \cdot \mathbf{S}_j)^2$ . The quartic term is excluded in this limit because it corresponds to second order perturbation theory in  $\gamma^{-1}$ . The prefactor in front of the spin-1 coupling can be determined thanks to the calculation of a single matrix element, which is easily done on the all-spin-up configuration and yields  $J_{\text{eff}} = J_{AF}/4$ .

If we consider a spin- $s$  antiferromagnetic spin chain with  $s$  even, characterized by the Hamiltonian  $\mathcal{H} = \sum_i J_{AF} \mathbf{S}_i \cdot \mathbf{S}_{i+1}$ , this spin chain can be mapped onto a NL $\sigma$ M. The mapping can be performed within the Lagrangian formalism if one uses coherent states representation for the spin operators. The discrete action is made of the exchange interaction terms and of the Berry phases  $W[\mathbf{n}_i]$  of the spin vector field  $\mathbf{n}_i$ . The coherent state vectors  $\mathbf{n}_i$  are expanded according to  $\mathbf{n}_{2i} = \mathbf{l}_{2i} - s\Phi_{2i}$ ,  $\mathbf{n}_{2i+1} = \mathbf{l}_{2i+1} + s\Phi_{2i+1}$ . The vector field  $\Phi_i$  (local staggered magnetization) is unitary and the field  $\mathbf{l}_i$  satisfies  $\Phi_i \cdot \mathbf{l}_i = 0$ . Those fields can be hinted at from the study of modes in the semi-classical spin chain. Now suppose  $\mathbf{l}_i$  is of order of magnitude  $a$ , the lattice spacing. This representation of the spin chain allows for a continuous form for the action  $S$ , which depends on the fields  $\mathbf{l}(x, t)$  and  $\Phi(x, t)$ . Because we supposed  $\mathbf{l}$  is of magnitude  $a$ , the action is quadratic in  $\mathbf{l}$  so that the field can be integrated out. Now recall that the spin magnitude  $s$  is even. Then the Berry phases of the spin coherent states partially gather to form a topological term  $\theta = 2\pi s$ , the effect of which is null in the action.

Let us consider now the alternating spin chain. The main difficulty we encounter in trying to represent this chain is the fact that it is inhomogeneous, so that writing an adequate continuous action out of the discrete Hamiltonian is not a trivial task. Indeed, the fundamental microscopic structure is a block of two spins (call them 1 and 2, say). It will turn out that it is better to choose pairs of spins naturally coupled by the ferromagnetic link, preferably to the antiferromagnetic one. This choice corresponds to the idea of pairing those spins  $s = 1/2$  to make them an effective spin-1 in the limit where  $\gamma$  goes to infinity (large ferromagnetic coupling).

The most rigorous way we could imagine to handle the continuous limit would be to introduce two coherent states vector fields, one for each of the two sites. Unfortunately, this would yield an intricate action, due to the appearance of several equally contributing massive modes. In particular, the Berry phases contribution of those coherent states would not be any more easily recognizable as a topological invariant.

Now consider a two-block structure, made of the four spins  $\mathbf{S}_{2i}^1, \mathbf{S}_{2i}^2, \mathbf{S}_{2i+1}^1$ , and  $\mathbf{S}_{2i+1}^2$ . The pairs  $\mathbf{S}_{2i}^1, \mathbf{S}_{2i+1}^1$  and  $\mathbf{S}_{2i}^2, \mathbf{S}_{2i+1}^2$  are appropriate candidates to generate two NL $\sigma$ M models. A first (incorrect) idea, sustained by our wish to go to the continuous limit, is to assume that they form the same NL $\sigma$ M. This assumption would be correct in the limiting case  $\gamma$  goes to infinity, but far too crude in any other case.

To cure this, at least partially, we add one extra field  $\Delta_i$  to the two semi-classical NL $\sigma$ M slow modes  $\mathbf{l}_i$  and  $\Phi_i$ . It represents small quantum fluctuations, remnants of

massive modes, that may bring about effective corrections to the NL $\sigma$ M action.

Accordingly, the coherent states fields are decomposed as:

$$\begin{cases} \mathbf{n}_{2i}^1 = \mathbf{l}_{2i} - s\bar{\Phi}_{2i} + a\Delta_{2i} \\ \mathbf{n}_{2i}^2 = \mathbf{l}_{2i} - s\bar{\Phi}_{2i} - a\Delta_{2i} \\ \mathbf{n}_{2i+1}^1 = \mathbf{l}_{2i+1} + s\bar{\Phi}_{2i+1} - a\Delta_{2i+1} \\ \mathbf{n}_{2i+1}^2 = \mathbf{l}_{2i+1} + s\bar{\Phi}_{2i+1} + a\Delta_{2i+1} \end{cases} \quad (2.2)$$

Here  $s$  is the spin magnitude and  $a$  is the lattice spacing. Note that this lattice spacing is of the length of a two-spin block. The amplitude of the quantum fluctuation is of the order of this lattice spacing. This assumption make the problem a tractable one, since we do not need to consider derivatives of the field  $\Delta_i$  when expanding the action. We enforce it by setting  $a$  as a prefactor of the fluctuating field. Note that the standard momentum field  $\mathbf{l}$  is implicitly assumed to be of order  $a$ .

We intentionally chose only one fluctuation field, contrary to S en echal's scheme [14] where the coherent state fields are decomposed on as many possible independent fluctuation fields. We now justify the choice of this particular field by means of a path integral reasoning.

We suspect that some highly fluctuating paths are contributing in the action. Indeed, exchange couplings vary on the microscopic scale by a macroscopic amount, and do not behave smoothly with respect to the position. As a consequence some irregular paths might be energetically favorable. Yet a straightforward continuous limit of the action would not retain them since they are not spatially regular. That is why we should enforce some possible (non derivable) contributing fluctuation in the paths. Now let us see why we chose this particular field  $\Delta_i$ . The fields  $\mathbf{l}_i$  and  $\bar{\Phi}_i$  parametrize the variation of the path between the two-block pattern  $(2i, 2i + 1)$ , spatially indexed by  $i$ . So we need one field to represent the variation inside the two-spin blocks. In the block  $2i$ , the coherent state vectors  $\mathbf{n}_{2i}^1$  and  $\mathbf{n}_{2i}^2$  differ by an amount of  $2a\Delta_i$ . Since the microscopic pattern is a two-spin block, we have then no choice than to make the coherent state vectors  $\mathbf{n}_{2i+1}^1$  and  $\mathbf{n}_{2i+1}^2$  differ by an amount of  $-2a\Delta_i$ , because the variation on the scale of the two-spin block are already taken into account within the NL $\sigma$ M fields. And this exhausts infinitesimal contributing fluctuations of the path.

The action of the spin chain we get through the coherent states representation is of the form

$$\begin{aligned} S = \int dt \sum_i s^2 \mathbf{n}_{2i} \cdot \mathbf{n}_{2i+1} \\ - \gamma \sum_i s^2 \mathbf{n}_{2i+1} \cdot \mathbf{n}_{2i+2} + \sum_i s \cdot W[\mathbf{n}_i]. \end{aligned} \quad (2.3)$$

One can expand the coupling terms in the action, then goes to the continuous limit, which yields

$$\begin{aligned} S_c = \int dt \frac{dx}{a} [-4a^2(1 + \gamma)\Delta^2 \\ - 4l^2 + 4a^2 s \partial_x \bar{\Phi} \cdot \Delta - a^2 s^2 (\partial_x \bar{\Phi})^2]. \end{aligned} \quad (2.4)$$

We emphasize the fact that the ferromagnetic exchange terms are of course expanded from its aligned configuration contrary to the antiferromagnetic exchange terms which are expanded from the N eel order. That is the reason why NL $\sigma$  models derived for antiferromagnetic ladder or alternating spin chain [16–19] cannot be straightforwardly applied to the present cases: they are not built upon the same semiclassical configurations. Note that since the measure element  $dx$  is a two-spin block, it is equal to  $a$ . The Berry phases of the spins are of the form  $\int dt dx \delta \mathbf{n} \cdot \mathbf{n} \wedge \partial_t \mathbf{n}$ , where  $\delta \mathbf{n}$  is the spatial variation of the field  $\mathbf{n}$ , and give

$$S_b = \int dt \frac{dx}{a} s(4\mathbf{l} + 2as\partial_x \bar{\Phi}) \cdot \bar{\Phi} \wedge \partial_t \bar{\Phi}. \quad (2.5)$$

Since we sum up the contributions for a double two-spin block, we must divide the whole sum by a factor 2. We end up with

$$\begin{aligned} S = \int dx dt \left[ -2(1 + \gamma)\Delta^2 - 2l^2 - 2s\Delta \cdot \partial_x \bar{\Phi} - \frac{1}{2}s^2(\partial_x \bar{\Phi})^2 \right] \\ + \int dx dt \left[ s^2(\partial_x \bar{\Phi}) \cdot \bar{\Phi} \wedge \partial_t \bar{\Phi} + 2s\mathbf{l} \cdot \bar{\Phi} \wedge \partial_t \bar{\Phi} \right], \end{aligned} \quad (2.6)$$

where we have set  $a = 1$  for commodity. We recover a spin- $2s$  topological  $\theta$ -term with  $\theta = 4\pi s$ . As a consequence, the topological term does not contribute, so that the spin chain is likely to be gapped.

We next integrate over the fluctuation fields, that is to say  $\mathbf{l}$  and  $\Delta$ . We then obtain the NL $\sigma$ M action

$$S = \int dt dx \left[ \frac{1}{2}(\partial_t \bar{\Phi})^2 - \frac{1}{2}s^2 \frac{\gamma}{1 + \gamma} (\partial_x \bar{\Phi})^2 \right]. \quad (2.7)$$

The standard parameters of this NL $\sigma$ M are the coupling constant  $g$  and the velocity  $c$  given by

$$g = \frac{1}{s} \sqrt{\frac{1 + \gamma}{\gamma}} \quad \text{and} \quad c = s \sqrt{\frac{\gamma}{1 + \gamma}}. \quad (2.8)$$

Note that  $c$  perfectly matches the velocity  $v$  we found for the classical spin waves. When we make  $\gamma$  goes to infinity the coupling constant  $g$  goes to  $1/s$  and the velocity goes to  $s$ . These are the expected parameters for the  $2s$ -NL $\sigma$ M. More precisely, the Hida's chain is build up of spin one half so that for  $s = 1/2$   $g$  goes to 2 and  $c$  to  $1/2$  in units of the antiferromagnetic exchange coupling. Those are the NL $\sigma$ M parameters of a spin-1 chain of exchange  $J_{AF}/4$ . This matches the limit found by Hida for the alternating chain, which we have recalled previously. Hence that in this limit, our NL $\sigma$ M is consistent with Hida's argument.

## 2.2 The gap formula

To evaluate the spin gap, we compute the mass generated by the NL $\sigma$ M in the limiting case of a large number of components for the field  $\bar{\Phi}$  ( $N \rightarrow \infty$ ). In that limit a closed expression can be obtained for it, thanks to the large  $N$  saddle-point approximation [22]. It leads to a dynamically generated mass, which is implicitly given by a

saddle point equation. Once one takes into account renormalization group corrections (effectively replacing  $N$  with  $N - 2$ ), and makes  $N = 3$ , one gets:

$$\int \frac{dk}{2\pi} \frac{d\omega}{2\pi} \frac{1}{\frac{c}{g}k^2 + \frac{1}{g}c\omega^2 + m^2} = 1. \quad (2.9)$$

At this point we must be cautious not to resort straightforwardly to the standard result for the mass. In the limit  $\gamma$  goes to 0, the chain is totally dimerized and the velocity  $c$  goes to 0. Because of this unusual feature, and also because we wish to derive results valid for a large range of  $\gamma$ , we will not resort to a radial cut-off in the Euclidean space-time of the NL $\sigma$ M. Rather we will first integrate on frequencies, then integrate on the momenta, with a large-momenta cut-off  $\Lambda$ . So that instead of the usual circular domain, we integrate over a strip in the plane  $(k, \omega)$  along the  $\omega$ -axis. The reason for this is that when  $\gamma$  goes to 0, the prefactor  $cg^{-1}$  of  $k^2$  goes also to zero whereas the prefactor  $(cg)^{-1}$  of  $\omega^2$  remains constant so that large frequencies are more and more relevant and must not be cut off. In the process (which actually corresponds to the decoupling of dimers), we lost the space dimension of space-time.

The first integration is over  $\omega$  and gives

$$g \int_{-\Lambda}^{\Lambda} \frac{dk}{4\pi} \frac{1}{\sqrt{k^2 + \frac{g}{c}m^2}} = 1. \quad (2.10)$$

Then integrating over  $k$  we can extract the mass of the NL $\sigma$ M

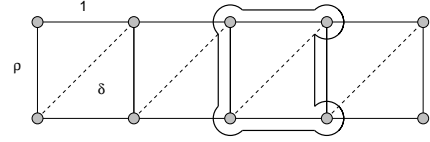
$$m = \sqrt{\frac{c}{g}} \frac{\Lambda}{\sinh(2\pi s \sqrt{\frac{\gamma}{1+\gamma}})}. \quad (2.11)$$

In the standard derivation of the mass generated by the NL $\sigma$ M (see for example [23]) one would exchange the function hyperbolic sine for the function exponential. Indeed, in order for this computation to make sense we must have  $\sqrt{gc^{-1}}m \ll \Lambda$ . Since in the NL $\sigma$ M related to the spin-2s chain,  $\sqrt{gc^{-1}}$  is finite, the (then meaningless) hyperbolic sine function can be replaced with the exponential function. Yet for our alternating chain, it can't be done since in the limit  $\gamma$  goes to 0 the argument of the function vanishes. Hence to encompass the full range of  $\gamma$  we must retain the hyperbolic sine function.

Now we can turn to the energy gap  $\Delta_{2s} = \sqrt{gcm}$ . Whatever the spin magnitude  $s$ , the gap of an antiferromagnetic pair of spins is equal to the gap between the triplet state and the singlet, *i.e.*  $J_{AF}$ . Hence when  $\gamma \rightarrow 0$ , we can determine that  $\Delta_{2s}$  goes to  $\Lambda/(2\pi)$ . This statement allows us to determine the cut-off which appears to be  $2\pi$  (actually  $2\pi/a$  but we set  $a = 1$ ). Therefore we can write:

$$\Delta_{2s} = \frac{2\pi s \sqrt{\frac{\gamma}{1+\gamma}}}{\sinh(2\pi s \sqrt{\frac{\gamma}{1+\gamma}})}. \quad (2.12)$$

We have obtained a *self-contained*, estimate of the chain gap for the spin magnitude  $s$ . For the spin-1 chain we



**Fig. 2.** A spin ladder with diagonal couplings  $\delta$ . The unit block to construct a NL $\sigma$ M contains again four spins.

obtain  $\Delta_1 = 4\pi/\sinh \pi$ , which is 1.08 far from the numerically [24] known 0.41. We expect a better result for the spin-2 chain, closer to the “large spin limit” where the saddle point approximation is accurate. We obtain  $\Delta_2 = 8\pi/\sinh 2\pi$ , which is 0.094 fairly close to the numerically [25] known value of 0.085. As for the correlation lengths, we obtain  $\xi_1 \sim 2$  to compare with the numerically known  $\xi_1 \sim 6$  whereas we obtained  $\xi_2 \sim 43$  to compare with the numerical value  $\xi_2 \sim 49$ .

The figures labeled 3 and 4 are drawings of the curves of the spin gap w.r.t.  $-\gamma$  in the range  $\gamma \in [0, 1]$  and  $-1/\gamma$  in the range  $\gamma \in [1, \infty[$ . We did so in order to compare our results to Hida’s presentation of his numerical computation [10]. Our result agrees qualitatively on the whole range of  $\gamma$  including the limiting case  $\gamma$  goes to zero.

To check that our NL $\sigma$ M approach is still valid in the limit  $\gamma$  goes to zero, we can also compute the correlation length. It can be read on the saddle point equation:  $\xi = \sqrt{\frac{c}{g}} \frac{1}{m}$ , or

$$\xi = \frac{1}{2\pi} \sinh \left( 2\pi s \sqrt{\frac{\gamma}{1+\gamma}} \right). \quad (2.13)$$

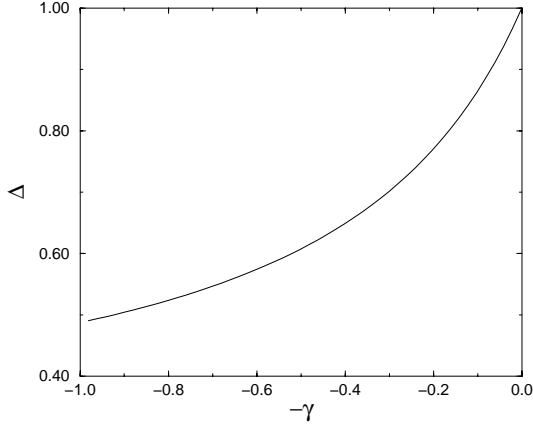
We check that the correlation length goes to zero like  $s\sqrt{\gamma}$  when  $\gamma \rightarrow 0$ , which is expected since at this point the chain is made of decoupled dimers.

### 3 An alternating spin ladder

In reference [15], White introduced several mappings that interpolate smoothly between spin ladders and a spin-1 chain within the Haldane’s spin gap phase. Here we treat one of these mappings. It consists in an antiferromagnetic spin ladder with an additional diagonal bond in every plaquette formed by legs and rungs (see Fig. 2). The exchange coupling associated to this bond is ferromagnetic (we will denote it as  $D$ ) and does not introduce any frustration in the ladder. The Hamiltonian is given by

$$\mathcal{H} = J \sum_{n;a=1,2} \mathbf{S}_n^a \mathbf{S}_{n+1}^a + K \sum_n \mathbf{S}_n^1 \mathbf{S}_n^2 + D \sum_n \mathbf{S}_n^1 \mathbf{S}_{n+1}^2 \quad (3.1)$$

where exchange couplings  $J$  and  $K$  are chosen positive, while  $D$  is negative. When  $D$  goes to 0 we recover the usual antiferromagnetic spin ladder. Whereas in the limit  $-D$  goes to infinity, the pairs of ferromagnetically bounded spin are in a triplet state. The effective Hamiltonian can then be expanded by rotational invariance in terms of spin-1 couplings. The effective antiferromagnetic coupling constant is then evaluated on any matrix element



**Fig. 3.** The gap of the alternating chain as a function of  $\gamma$ . The point with decoupled dimers is on the right.

of the Hamiltonian and gives  $J_{\text{eff}} = (2J + K)/4$ . So this limit corresponds to an antiferromagnetic spin-1 chain. Since in the process, the ladder remains in the Haldane gapped phase, we may apply our scheme to obtain an estimate of the gap as a function of the diagonal coupling  $D$ .

### 3.1 Effective NL $\sigma$ M

The microscopic pattern of the ladder is composed of the four spins  $\mathbf{S}_{2i}^1, \mathbf{S}_{2i}^2, \mathbf{S}_{2i+1}^1$ , and  $\mathbf{S}_{2i+1}^2$  forming a square and, apart from the additional diagonal bond, three bonds: one on each leg, and the last one on one of the two rungs closing the square (see Fig. 2). As for the Hida's chain case calculations are done on a doubled cell.

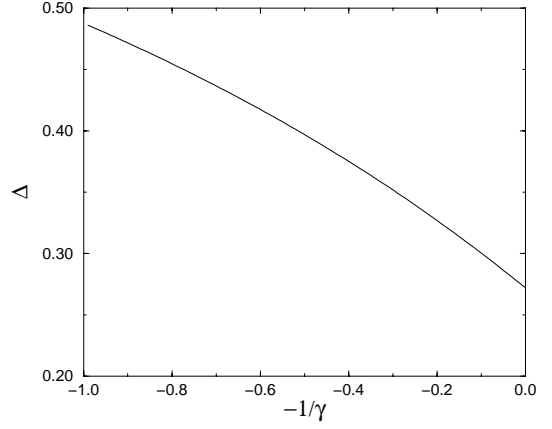
Possible candidates to spin pairs forming a NL $\sigma$ M are the nearest neighbours on the same leg. Pairs of site linked by a rung contribute to the same NL $\sigma$ M. Then, we will need only one extra fluctuation field to describe of fluctuating paths inside the elementary cell, *before* going to the continuous limit. Accordingly the coherent states fields are decomposed as:

$$\begin{cases} \mathbf{n}_{2i}^1 = \mathbf{l}_{2i} - s\Phi_{2i} + a\Delta_{2i} \\ \mathbf{n}_{2i}^2 = \mathbf{l}_{2i} - s\Phi_{2i} + a\Delta_{2i} \\ \mathbf{n}_{2i+1}^1 = \mathbf{l}_{2i+1} + s\Phi_{2i+1} - a\Delta_{2i+1} \\ \mathbf{n}_{2i+1}^2 = \mathbf{l}_{2i+1} + s\Phi_{2i+1} - a\Delta_{2i+1} \end{cases} \quad (3.2)$$

In the following we set  $J = 1$ ,  $K = \rho$  and  $D = -\delta$  so that the coupling constants are expressed in units of the longitudinal antiferromagnetic coupling  $J$ . One can then expand the coupling terms in the action, which yields:

$$S_c = \int dt \frac{dx}{a} [-4a^2(\rho + \delta)\Delta^2 - 4(2 + \rho)\mathbf{l}^2 + 4a^2\delta s \partial_x \Phi \cdot \Delta - a^2(\rho + \delta)s^2(\partial_x \Phi)^2] \quad (3.3)$$

with the same care for the ferromagnetic bonds as was done previously. Like for the Hida's chain the measure element  $dx$  is a two-spin block and is equal to  $a$ . The Berry



**Fig. 4.** Same as preceding figure but the  $S = 1$  chain is recovered on the right for  $1/\gamma = 0$ .

phases of the spins are of the form  $\int dt dx \delta \mathbf{n} \cdot \mathbf{n} \wedge \partial_t \mathbf{n}$  and give

$$S_b = \int dt \frac{dx}{a} 2s \mathbf{l} \cdot \Phi \wedge \partial_t \Phi. \quad (3.4)$$

Since we sum up the contributions for a double two-spin block, we must divide the whole sum by 2. We end up with:

$$S = \int dx dt [-2(2 + \rho)\mathbf{l}^2 - 2(\rho + \delta)\Delta^2 - 2s\Delta \cdot \partial_x \Phi - \frac{1}{2}s^2(2 + \delta)(\partial_x \Phi)^2] + \int dx dt [2\mathbf{l}s\Phi \wedge \partial_t \Phi] \quad (3.5)$$

where we have set  $a = 1$ . We next integrate over the fluctuation fields, that is to  $\mathbf{l}$  and  $\Delta$ . So that we finally obtain the NL $\sigma$ M action

$$S = \int dt dx \left[ \frac{1}{2 + \rho} (\partial_t \Phi)^2 - \frac{1}{2} s^2 (2 + \frac{\delta\rho}{\delta + \rho}) (\partial_x \Phi)^2 \right]. \quad (3.6)$$

The standard parameter of this NL $\sigma$ M are

$$g = \frac{1}{s} \sqrt{\frac{2 + \rho}{2 + \frac{\delta\rho}{\delta + \rho}}} \quad \text{and} \quad c = s \sqrt{(2 + \rho) \left( 2 + \frac{\delta\rho}{\delta + \rho} \right)}. \quad (3.7)$$

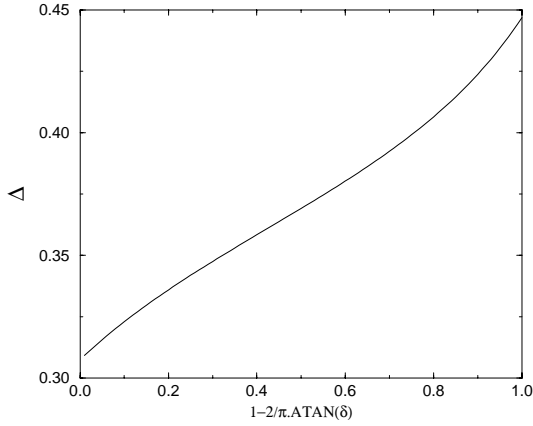
Now in order to stick to White's notations, we set  $\rho = 1$  to get:

$$g = \frac{1}{s} \sqrt{\frac{3(1 + \delta)}{2 + 3\delta}} \quad c = \frac{s}{2} \sqrt{\frac{3(2 + 3\delta)}{1 + \delta}}. \quad (3.8)$$

These are the coupling and the velocity of the effective NL $\sigma$ M.

### 3.2 Gap evaluation

A line of reasoning similar to the previous treatment can be applied to this NL $\sigma$ M. Contrary to the Hida's chain



**Fig. 5.** The gap of the spin ladder with diagonal couplings as a function of  $1 - 2/\pi \arctan(\delta)$ .

case, it is not meaningful to retain the hyperbolic sine function, since it is not more precise than the standard form for the gap. With the previously computed coupling constant  $g$  and velocity  $c$ , we obtain:

$$\Delta_L^s = A \frac{s}{2} \sqrt{\frac{3(2+3\delta)}{1+\delta}} \exp\left(-2\pi s \sqrt{\frac{2+3\delta}{3(1+\delta)}}\right). \quad (3.9)$$

Since when  $\delta \rightarrow \infty$ , we should recover  $3/4$  of the gap  $\Delta_C$  of the spin-1 chain, we can rewrite it as:

$$\frac{\Delta_L^s}{\frac{3}{4}\Delta_C} = \sqrt{\frac{2+3\delta}{3(1+\delta)}} \exp\left[2\pi s \left(1 - \sqrt{\frac{2+3\delta}{3(1+\delta)}}\right)\right]. \quad (3.10)$$

Hence we can relate the spin gap of the antiferromagnetic spin-1 chain to the spin gap of the antiferromagnetic two-leg spin 1/2 ladder by the formula:

$$\frac{\Delta_L}{\Delta_C} = \sqrt{\frac{3}{8}} \exp\left[\pi \left(1 - \sqrt{\frac{2}{3}}\right)\right]. \quad (3.11)$$

With the value  $\Delta_C \simeq 0.41$ , we obtain the estimate  $\Delta_L \simeq 0.45$ , close to the known [26] value 0.50. In Figure 5, we have drawn the curve of the normalized spin gap  $\Delta_L/(3/4\Delta_C)$  w.r.t.  $1 - 2/\pi \arctan \delta$ . We can compare the curve with data from White [15]. Not only does our result agree qualitatively, but it is also quantitatively quite good.

## 4 Conclusion

We have constructed non-linear sigma models appropriate to the description of the properties of some generalized spin chains including ferromagnetic exchanges. In the case of the alternating ferro-antiferromagnetic spin chain, our treatment reproduces correctly the smooth crossover from decoupled dimers to the Haldane phase. This approach may be of relevance to the study of the compound  $\text{CuNb}_2\text{O}_6$  which is such an alternating chain and has a spin gap [27].

We have also treated a ladder including ferro bonds so that the Haldane phase can be reached. Here again there is good agreement with numerical data.

We thank A.V. Chubukov for useful discussions and collaboration at an early stage of this work.

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