#### SPIN-S ANTIFERROMAGNETIC CHAIN: AN ANALYTICAL STUDY

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We study the long wavelength limit of a spin-*s* Heisenberg antiferromagnetic chain with nearest neighbour interaction, via the nonlinear  $\sigma$  model (NL $\sigma$ M). We show by mean of Liouville theorem, that the topological term emerges naturally during the passage to a continuum limit field theory. The difference between bosonic and fermionic chains emerges only after the Heisenberg model is mapped onto a NL $\sigma$ M. The latter is developed further and tested for Heisenberg Hamitonian with first and second neighbour coupling, using Non abelian bosonization and renormalization group argument. This gives a qualitative explanation of the so-called Haldane's conjecture.

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# 1 Introduction

The discovery of high-temperature superconductivity has led to a great theoretical and experimental interest in understanding low-dimensional Heisenberg antiferromagnets (HAF) [1–3], partly because of the widespread belief that magnetism plays a key role in high-temperature superconductivity, but also because of the successful application of field-theoretical approaches to these systems, in particular to spin chains. Indeed, in 1983 Haldane conjectured that in the case of integer spin, the spin-s quantum HAF chain has a unique disordered ground state with a finite excitation gap, while the same model has no excitation gap when s is a half-odd-integer [4]. Using a mapping to the NL $\sigma$ M, valid in the large-s limit, the origin of the difference has been identified as being due to an extra topological " $\Theta$  term" in the effective  $\sigma$ -model Lagrangian for systems with half-integer s [4]. This clearly suggests that the origin of this difference is nonperturbative. At the beginning this came as a surprise, since for the half-integer-spin 1D HAF the excitation spectrum was known to be gapless. Very soon Haldanes conjecture was confirmed by many numerical and experimental studies [5] and the Haldane gap phenomenon is by now rather well understood. However, such a mapping may be termed semiclassical, since it is constructed by introducing a local field characterizing the order expected in the classical ground state and by taking into account fluctuations of the spin variables around this local order.

In the present work, we study a simple HAF chain by the use of Affleck's prescription [6, 7]. The main result of our approach is that contrary to Affleck's [8], we show by mean of Liouville theorem, that the topological term is naturally deduced. We also obtain, with the help

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of bosonization technique and renormalization group analysis, an effective theory for the lowenergy physics of s = 1/2 spin chains with nearest and next nearest neighbour coupling and a reconfirmation of Haldane's conjecture.

The organization of this paper will be as follows. In section II, our discussion so far of the antiferromagnetic chain will be fully classical and will involve an approach based on the large-spin, semiclassical limit. In this approach one approximates the field of spin site operators  $\mathbf{S}_i \left[\mathbf{S}_i^2 = s(s+1)\right]$ , retaining only the Fourier components near  $k_x = 0$ , and  $\pi$  (Haldane mapping), then taking the continuous limit. Moreover, the one-dimensional Heisenberg model will be mapped onto a NL $\sigma$ M field theory along the following lines: the continuum limit of the Hamiltonian is taken; then new variables are introduced to facilitate the calculation of the Lagrangian and thus of the (dynamic) action. In section III, we examine the Heisenberg model with nearest and next nearest coupling and discuss the Haldane conjecture using Non abelian bosonization formalism. Section V contains our conclusion. Appendix A and B, respectively give a brief description of the fermionic coset version of the level-1 WZW theory and the calculation of the spin correlation function.

## 2 Continuum description of a single spin chain

#### 2.1 Definition of a continuous field theory in one-dimensional case

Consider an individual 1D HAF chain of spins. In the case of a nearest-neighbour interaction, the Hamiltonian is given by

$$H_{\text{Heisenberg}} = J \sum_{i} \mathbf{S}_{i} \cdot \mathbf{S}_{i+1} \tag{1}$$

where S is an operator which represents the local degree of freedom, satisfying the Poisson brackets

$$\left\{S_i^a, S_j^b\right\} = i\varepsilon^{abc}S_j^c\delta_{ij}.$$
(2)

In the classical limit (large S) and when looking for low-energy excitations, we can introduce a local field characterizing the order and take into account fluctuations of the spin variables around this local order. In the case of the simple AF chain, a collinear order exists in the classical ground state and the local field introduced is a unit vector  $\mathbf{n}(x)$ , representing the staggered magnetization. Under this assumptions,  $\mathbf{S}_{2i} + \mathbf{S}_{2i+1}$  will be small (of the order of  $a_0$ , the lattice spacing). Following Affleck [8], we can introduce an elementary cell of size  $2a_0$  (it now includes two spins). According to Haldane [4] prescription, we shall decompose the original order parameter into a slow varying mode  $\mathbf{n}(x)$  such that

$$\mathbf{n}(x) = \frac{1}{2\nu} (\mathbf{S}_{2i} - \mathbf{S}_{2i+1}), \tag{3}$$

and a local magnetization l(x), associated with a rapidly varying mode such that

$$\mathbf{l}(x) = \frac{1}{2a_0} (\mathbf{S}_{2i} + \mathbf{S}_{2i+1}), \tag{4}$$

with  $\nu = \sqrt{s(s+1)}$ . These two fields correspond to the Fourier modes of the spin operators, with momenta near (q = 0) and  $(q = \pi)$ . Firstly, we notice that the low energy degrees of freedom occur at wave-vectors near 0 and  $\pi$  (this can be seen from spin-wave theory, for example, even though spin wave theory is not correct in detail) and a formal justification for *only* keeping Fourier modes near these wave-vectors is provided by the renormalization group: one can integrate out the high energy degrees of freedom to derive an effective Lagrangian for the low energy degrees of freedom. This is a rather standard approach to many problems in critical phenomena and high energy physics. Secondly, the transformation (3, 4) to the  $\sigma$ -model degrees of freedom is useful because some insights about the behavior of the  $\sigma$ -model are available.

In the classical limit, the Casimir operator  $S^2$  imposes between the new local antiferromagnetic degrees of freedom the following true relations

$$\mathbf{n}^2 = 1 - \frac{a^2}{\nu^2} \mathbf{l}^2$$
  
$$\mathbf{n} \cdot \mathbf{l} = 0.$$
 (5)

These two constraints ensure that there are four independent variables per unit cell  $(2a_0)$ . This clearly shows that the total number of degrees of freedom (equals to 4) is conserved. Strictly speaking, we have associated to each site *i* of lattice a spin operator  $S_i^{\alpha}$  which generate a Lie algebra (2) with usual notations. Long distance magnetic behaviour may be tackled applying a prescription due to Affleck [6,7]: one tends conjointly the step  $a_0$ , the quantum number *s* to zero and infinity respectively while maintaining constant measurable physical entities. In this respect spins are implicitly treated in the classical limit since the commutation relation (2), which to have a physical sense must be written as

$$\left\{\frac{S_i^a}{s}, \frac{S_j^b}{s}\right\} = \frac{1}{s^2} \mathrm{i}\varepsilon^{abc} S_i^c \delta_{ij} \tag{6}$$

vanishes when s approaches infinity. Therefore, in the continuum limit where  $\lim_{a_0 \to 0} \frac{\delta_{x_1,x_2}}{2a} = \delta(x_1 - x_2)$ , the new degrees of freedom generate simple Poisson brackets

$$\{l^{i}(x_{1}), l^{j}(x_{2})\} = i\varepsilon^{ijk}l^{k}\delta(x_{1} - x_{2}) \{l^{i}(x_{1}), n^{j}(x_{2})\} = i\varepsilon^{ijk}n^{k}\delta(x_{1} - x_{2}) \{n^{i}(x_{1}), n^{j}(x_{2})\} = i\frac{4a_{0}^{2}}{\nu^{2}}\varepsilon^{ijk}l^{k}\delta(x_{1} - x_{2}) \to 0.$$

$$(7)$$

Thus we conclude that the order parameter **n** is a free field of tridimensional vectors, of length one. Moreover, the SO(3) Lie algebra structure generated by the Poisson Brackets for l indicates that this field is the generator of rotations: the spin density l behaves like an angular momentum in the continuum limit.

### 2.2 Semiclassical mapping to nonlinear $\sigma$ -model

In this subsection we argue that the long-wavelength, continuum theory describing a simple AF spin chain is specified by the Lagrangian of Eq. (16), with notation explained thereafter. The derivation of the angular momentum will be the starting point.

## 2.2.1 The angular momentum

In addition to (5), the Liouville theorem

$$\frac{\partial \mathbf{S}_i}{\partial t} = i \left\{ \mathbf{H}, \mathbf{S}_i \right\},\tag{8}$$

allows us to establish another relation between l and n. We apply it to  $S_{2i}$  and  $S_{2i+1}$  successively, since for the AF case it is more appropriate to write down the equations for the spin vectors at the even and odd sites (regarded as two sublattices) separately as follows:

$$\frac{d\mathbf{S}_{2i}}{dt} = J\mathbf{S}_{2i} \times (\mathbf{S}_{2i-1} + \mathbf{S}_{2i+1})$$
  
$$\frac{d\mathbf{S}_{2i+1}}{dt} = J\mathbf{S}_{2i+1} \times (\mathbf{S}_{2i} + \mathbf{S}_{2i+2}), \qquad (9)$$

now by reversing the relationships (3), (4), the old degrees of freedom read

$$\mathbf{S}_{2i} = \nu \mathbf{n} + a_0 \mathbf{l}$$
  

$$\mathbf{S}_{2i+1} = -\nu \mathbf{n} + a_0 \mathbf{l},$$
(10)

and the dynamics of the free field n is given by

$$2\nu \frac{\partial \mathbf{n}}{\partial t} = \frac{d\mathbf{S}_{2i}}{dt} - \frac{d\mathbf{S}_{2i+1}}{dt}$$
  
=  $J(\mathbf{S}_{2i-1} + \mathbf{S}_{2i+1}) \times \mathbf{S}_{2i} - J(\mathbf{S}_{2i} + \mathbf{S}_{2i+2}) \times \mathbf{S}_{2i+1}$   
=  $J\mathbf{S}_{2i-1} \times \mathbf{S}_{2i} + 2J\mathbf{S}_{2i+1} \times \mathbf{S}_{2i} - J\mathbf{S}_{2i+2} \times \mathbf{S}_{2i+1}$  (11)

$$2\frac{\partial \mathbf{n}}{\partial t} = J \left[ -\mathbf{n}(x - 2a_0) + \frac{a_0}{\nu} \mathbf{l}(x - 2a_0) \right] \times \left[ \mathbf{n}(x) + \frac{a_0}{\nu} \mathbf{l}(x) \right] + \frac{4Ja_0}{\nu} \mathbf{l}(x) \times \mathbf{n}(x) - J \left[ \mathbf{n}(x + 2a_0) + \frac{a_0}{\nu} \mathbf{l}(x + 2a_0) \right] \times \left[ -\mathbf{n}(x) + \frac{a_0}{\nu} \mathbf{l}(x) \right]$$
(12)

When expanding the order parameter **n** in the neighbourhood of x (the center of elementary cell) using appropriate Taylor expansion for  $l(x \pm 2a_0)$  and  $n(x \pm 2a_0)$ , we can write

$$\frac{1\partial \mathbf{n}(\mathbf{x})}{2Ja\partial t} = 2\mathbf{l}(x) \times \mathbf{n}(x) - \nu \mathbf{n}(x) \times \partial_x \mathbf{n}(x)$$
(13)

The *cross product* of the free field  $\mathbf{n}$  and expression (13) can be performed, then the angular momentum can be written by taking into account the constraints (5) as follows

$$\mathbf{l} = \mathbf{n} \times \mathbf{\Pi} = \mathbf{n} \times \frac{\partial \mathbf{n}}{cg^2 \partial t} - \frac{\Theta}{4\pi} \partial_x \mathbf{n}(\mathbf{x}).$$
(14)

Here  $\mathbf{\Pi}$  is the momentum conjugate to  $\mathbf{n}$  satisfying

$$\{\pi^{i}(x_{1}), \pi^{j}(x_{2})\} = 0 \{n^{i}(x_{1}), \pi^{j}(x_{2})\} = i\delta_{ij}\delta(x_{1}-x_{2}),$$
 (15)

the dimensionless coupling constant g, measuring the strength of quantum fluctuations, and the velocity of magnons c are related to the spin s, the AF coupling J, and the lattice spacing  $a_0$ :  $c = 2Ja_0s$  and  $g^2 = 2/s$ . We have also defined  $\Theta = 2\pi s$ .

According to Eq. (14), the field l contains two terms. In addition to the generator of rotations associated with the observables degrees of freedom (the order parameter of n), the Liouville theorem reveals naturally an additional term. We also note that it does not result from an identification *a posteriori* as in Affleck [8]. We either did not add an *ad-hoc* additional term as Shankar and Read [2].

### 2.2.2 Calculating action

If we expand Heisenberg Hamiltonian (1) as a function of the variables l, n and  $\frac{\partial n}{\partial t}$ , we get

$$H_{\text{Heisenberg}} = a_0 c \sum_i g^2 \left[ \mathbf{l}^2 + \nu \mathbf{l}(x) \cdot \partial_x \mathbf{n}(x) + \frac{\nu^2}{4} (\partial_x \mathbf{n}(x))^2 \right] + \frac{1}{g^2} (\partial_x \mathbf{n}(x))^2.$$
(16)

In the limit where  $a_0$  goes to  $0, 2a_0 \sum_i \rightarrow \int dx$ . Therefore, we can write

$$H_{\text{Heisenberg}} = \frac{c}{2} \int \left( g^2 \left[ 1 + \frac{\Theta}{4\pi} \partial_x \mathbf{n}(x) \right]^2 + \frac{1}{g^2} (\partial_x \mathbf{n}(x))^2 \right) \mathrm{d}x.$$
(17)

If we replace  $\mathbf{l}$  with expression (14), we find

$$H = \frac{1}{2g^2} \int \left[ \frac{1}{c} (\partial_t \mathbf{n})^2 - c (\partial_x \mathbf{n})^2 \right] \mathrm{d}x.$$
(18)

Thus, the long-distance behaviour of the infinite one-dimensional chain of Heisenberg spin is given by the NL $\sigma$ M. As  $\mathbf{n}^2 = 1$ , we can express it as a function of the coordinates of the sphere  $(\theta, \varphi)$ . The angular momentum l then writes

$$\mathbf{l} = \mathbf{n} \times \left[ \pi_{\theta} \frac{\partial \mathbf{n}}{\partial t} + \frac{1}{\sin^2 \theta} \pi_{\varphi} \right],\tag{19}$$

where the conjugate momenta are

$$\pi_{\theta} = \frac{\partial \theta}{cg^{2}\partial t} - \frac{\Theta}{4\pi} \sin \theta \partial_{x} \varphi$$
  
$$\pi_{\varphi} = \frac{\sin^{2} \theta \partial \varphi}{cg^{2}\partial t} + \frac{\alpha}{4\pi} \sin \theta \partial_{x} \theta.$$
 (20)

A Legendre transformation:  $\mathcal{L} = \pi_{\theta} \partial_t \theta + \pi_{\varphi} \partial_t \varphi - \mathcal{H}$  (here  $\mathcal{H}$  is the Hamiltonian density), using the conjugate momenta given by the relation (20), leads, for this system, to the following Lagrangian

$$L_{1+1} = \frac{1}{2g^2} \int \int \left[ \frac{1}{c} (\partial_t \mathbf{n})^2 - c(\partial_x \mathbf{n})^2 \right] dx dt + c \frac{\Theta}{4\pi} \sin \theta \left( \partial_x \theta \partial_t \varphi - \partial_t \theta \partial_x \varphi \right).$$
(21)

This is just  $NL\sigma M$  Lagrangian plus a"  $\Theta$  term" which is a total derivative and purely topological, and so has no effect on the classical equations of motion, as well as in perturbation theory. It does however, determines the statistical of excitations. It permits to generate a different statistics for excitations constructed from integer spins and for those constructed from half-integer spins, and hence provides a microscopic explanation for the Fermi-Bose transmutation [9]. Now, to understand better what this term represents, we notice that it is constructed from the topological current density

$$\mathbf{J} = \sin\theta d\theta \times d\varphi 
= \sin\theta \left(\partial_x \theta \partial_t \varphi - \partial_t \theta \partial_x \varphi\right).$$
(22)

Such a term, in fact, is simply the Jacobian of the coordinates transformation  $(\theta, \varphi) \rightarrow (x, y)$ . Defining the topological charge

$$Q = \int \int \mathbf{J} d\mathbf{S}$$
  

$$Q = \int \int \mathbf{J} dx dt,$$
(23)

this is then an integer  $(Q \in \mathbb{N})$ , since it is the topological number corresponding to the mapping of the two-dimensional sphere into the gauge group SU(2).

The final conclusion is that the topological term, is proportional to an integer Q. Then the action in the path-integral has a contribution equal to  $\Theta Q = (2\pi s)Q$  which should be added to the sigma-model term. As s can be an integer or a half-integer, we see that the extra topological term gives contribution:  $e^{i2\pi Q} = (-1)^{2sQ}$ . So if s is an integer (e.g., s = 1, then  $\Theta = 2\pi$ ) the spin chain is described at low energies by the NL $\sigma$ M. For a half-integer s (e.g., s = 1/2, then  $\Theta = \pi$ ), each topological class contributes with a sign which is positive (negative) if the topological charge Q is even (odd). The topological term seems to induce different qualitative behaviour for bosonic Heisenberg chains on one hand and fermionic chains on the other. This property implies a very important result, known as Haldane's conjecture which states that: The integer spin chains are massive (*i.e* have a gap) while the half-integer chains are massless (e.g spin 1/2 case). The latter statement may be studied by means of Non-abelian bosonization technique.

### 3 Look at the Haldane conjecture from the bosonization point view

From the Bethe ansatz solution [10], we know that the Hamiltonian (1) is critical. This means that the zero temperature spin correlators have power-law decays in both space and time (see Appendix B), over a finite range of ratios of short-range exchange interactions. It was also argued by Affleck and Haldane [11] that this critical point is well described by a level-1 Wess-Zumino-Witten (WZW) conformal field theory. This equivalence is demonstrated by starting from the half-filled Hubbard<sup>2</sup> model with hopping integral t and on-site repulsion U and taking the continuum limit. The charge degrees of freedom are then described by a Bose field  $\varphi$  which becomes massive for arbitrary small U, while the spin degrees of freedom are described by the level-1 WZW model. Now, we shall review this in details and extend the somewhat brief theoretical analysis of ref [11].

 $<sup>^{2}</sup>$ Since the Heisenberg model is derived from the second order perturbation expansion in strong coupling limit of Hubbard model.

## 3.1 The continuum field theory description of the Hubbard model in one dimension

The Hubbard model describes the dynamics of non-relativistic electrons moving on a lattice. Its Hamiltonian consists of a kinetic hopping term of strength t, and an on-site repulsion between up and down spins of strength U modeling the Coulomb interaction. At infinite U, one must pay infinite energy to put two electrons of opposite spins in the same point. Hence, double occupancy is strictly forbidden, and the electrons can move in the lattice only if some sites are vacant. Consequently, at half-filling, i.e. when the number of electrons equals the number of lattice points, the infinite U Hubbard model describes an insulator (of the Mott type [12]). Notice that this insulating behavior occurs at half-filling, while ordinary insulators are always characterized by completely filled bands. Applied to the square lattice, this model may well provide an explanation for high-temperature superconductivity [13]

We now recall the derivation of Hubbard Hamiltonian in the infrared limit. We begin with the free Hamiltonian and then treat the interaction case.

#### 3.1.1 Free theory

We start with the Hubbard Hamiltonian in one dimension which has the well-known form

$$H = t \sum_{i,\alpha} \left( c^{\dagger}_{\alpha,i} c_{\alpha,i+1} + c^{\dagger}_{\alpha,i+1} c_{\alpha,i} \right) + U \sum_{i} n_{\uparrow,i} n_{\downarrow,i}$$
(24)

where  $c_{\alpha i}$  is the fermion annihilation operator on site *i* with spin  $\alpha$ ,  $n_{\alpha i}$  is the corresponding number operator. We first consider the case without interaction (U = 0). In the reciprocal space, the free Hamiltonian is

$$H^{0} = \sum_{k,s} \varepsilon(k) c_{\alpha}^{\dagger}(k) c_{\alpha}(k), \qquad (25)$$

where  $\varepsilon(k)$  is the single-particle bandstructure. The dispersion relation is  $\varepsilon_k = -t \cos ka_0$ . Here, the Fermi surface consists just of two points  $\pm k_F$  and for weak interactions between the particles, only states in the immediate vicinity of the Fermi points are important. For these states, one can linearize the electronic dispersion relation around the Fermi points and take the continuum limit, considering *only* the degrees of freedom with low energy, at  $\pm v_F \Lambda$  of the Fermi level, where  $\Lambda$ is a cut-off on the wave vector which are relative to the Fermi surface  $(\pm k_F)$ . In this case, the theory is expressed in terms of right and left going excitations  $\psi_{R\alpha}, \psi_{L\alpha}$ , which both move with the Fermi velocity through the system. The continuum limit is obtained by factoring out the  $k_F$ dependance of the fermions field

$$c_{\alpha}(x) = \sqrt{a_0} \left( \psi_{R\alpha}(x) e^{\mathrm{i}k_{\mathrm{F}}x} + \psi_{L\alpha}(x) e^{-\mathrm{i}k_{\mathrm{F}}x} \right), \tag{26}$$

where  $\psi_{R\alpha}(x)$ ,  $\psi_{L\alpha}(x)$  are slowly varying fields of the variables x and  $a_0$  is the lattice constant. Because c(x) is dimensionless,  $\psi_R$  and  $\psi_L$  have scaling dimension 1/2. Moreover, as soon as x becomes a continuous variables, the canonical anticommutation relations

$$\{\psi \dagger_{R, L}(x), \psi_{R, L}(x')\} = \delta(x - x'), \tag{27}$$

becomes compatible with the ones of the lattice fermions

$$\left\{c_{n}^{\dagger}, c_{m}\right\} = \delta_{n, m}. \tag{28}$$

Expanding (25) in terms of the right- and left-moving fields in (26), results in

$$H^{0} = v_{\rm F} \int \mathrm{d}\sigma \psi_{R}^{\dagger}(x) \mathrm{i}\partial_{x}\psi_{R}(x) - \psi_{L}^{\dagger}(x)\mathrm{i}\partial_{x}\psi_{L}(x), \qquad (29)$$

where  $v_{\rm F} = \partial \varepsilon(k_{\rm F})/\partial k = a_0 \sin(k_{\rm F} a_0)$ . The right-hand side of (29) is exactly the Hamiltonian for massless relativistic Dirac fermions. In deriving (29), we first neglect the fast varying fields with prefactors  $\exp(\pm 2ik_{\rm F}x)$ , because these processes have a negligible probability and  $2k_{\rm F}$ is not a vector of the reciprocal lattice. We note that in the presence of a dimerization, these processes are no longer negligible, because  $2k_{\rm F}$  is a reciprocal lattice vector. Second, we consider x as a continuous variable. Third, we expand  $\psi^{\dagger}_{R, L}(x + a_0) = \psi^{\dagger}_{R, L}(x) + a_0 \partial_x \psi^{\dagger}_{R, L}(x)$  and neglect the higher-order derivatives, which do not contribute to the infrared limit. Fourth, we drop the constant ground state. The free Hamiltonian is then diagonalized via a bosonization procedure [14]. This requires to introduce the following operators  $(n \in \mathbb{Z})$ 

$$\mathcal{J}_{n} = \int \mathcal{J}^{0}(x)e^{-iK\cdot x} dx$$
  
$$\overline{\mathcal{J}}_{n} = \int \overline{\mathcal{J}}^{0}(x)e^{iK\cdot x} dx,$$
(30)

where

$$\mathcal{J}^{0}(x) = \psi_{R}^{\dagger}(x)\psi_{R}(x),$$
  

$$\overline{\mathcal{J}}^{0}(x) = \psi_{L}^{\dagger}(x)\psi_{L}(x).$$
(31)

We can now show that modes (30) satisfies the commutative relations  $[\mathcal{J}_n, \mathcal{J}_m] = n\delta_{n,-m}\mathbf{1}$ . These two relations define the infinite-dimensional Heisenberg algebra [15], also called the affine U(1) algebra denoted by  $\hat{U}(1)$ . Therefore, the symmetry of the model is given by two commuting copies of Heisenberg algebra<sup>3</sup>. The vacuum state of the Dirac theory,  $|0\rangle$ , satisfies the highest-weight condition, which implement the Pauli exclusion principle  $\forall n > 0$ ,  $\mathcal{J}_n^0 |0\rangle = \overline{\mathcal{J}}^0 |0\rangle = 0$ . Finally, as shown by Haldane [14], the free Hamiltonian can be expressed in terms of the currents

$$H^{0} = \pi v_{\rm F} \int \left( \mathcal{J}^{0}(x)^{2} + \overline{\mathcal{J}}^{0}(x)^{2} \right) \mathrm{d}x, \tag{32}$$

which is precisely the boson Hamiltonian, after using [16]  $\mathcal{J}^0 = \frac{i}{\sqrt{\pi}} \partial \phi$  and  $\overline{\mathcal{J}}^0 = -\frac{i}{\sqrt{\pi}} \partial \phi$ .

### **3.1.2** Interaction theory

Before we come to the interaction case, we shall note that for the half-filled band Hubbard model, the number of fermions per site is exactly one, so the charge degrees of freedom are frozen. In the conformal limit, this constraint is equivalent to the condition

$$\mathcal{J}_n | phys \rangle = 0, \ n \ge 0, \tag{33}$$

<sup>&</sup>lt;sup>3</sup>This factorization in a left and a right symmetry algebra is usual in CFT.

where  $\mathcal{J}_n$  is the U(1) fermionic current. The such constrained model provides a representation of  $SU(N)_1$ -WZW as a fermionic coset model (see Appendix A).

We now consider the effect of the Hubbard interaction U and then we bosonize. The most elegant way of doing this is to use Witten's non-Abelian bosonization [16]. This non-Abelian bosonization expresses a set of fermion fields in terms of a matrix field g belonging to a representation of a Lie algebra, instead of one or more simple boson fields and for SU(2) case, it may be introduced starting with the various components of the spin currents  $\mathcal{J}^a(a = 1, 2, 3)$  defined in terms of two electron fields

$$\mathcal{J}^{a} = \psi^{\dagger}_{R\alpha} \frac{\sigma^{a}_{\alpha\beta}}{2} \psi_{R\beta}$$
$$\overline{\mathcal{J}}^{a} = \psi^{\dagger}_{L\alpha} \frac{\sigma^{a}_{\alpha\beta}}{2} \psi_{L\beta}$$
(34)

( $\sigma^a$  being the usual Pauli matrices). Likewise, the g-field and its adjoint are given by [17]

$$g_{\alpha\beta} = \psi_{R\alpha}^{\dagger}\psi_{L\beta}$$

$$(g^{\dagger})_{\alpha\beta} = \psi_{L\alpha}^{\dagger}\psi_{R\beta}$$
(35)

In the language of conformal field theory, g is the spin-1/2 primary field of  $SU(2)_{2s}$  WZW theory,  $\Phi^{\frac{1}{2}}$ , with conformal dimension  $h = \overline{h} = \frac{3}{[8(s+1)]}$ . Using (26), (31), (34) and (35), we can write the continuum expressions of the charge and

spin density operators

$$n(x) = c^{\dagger}_{\alpha}(x)c_{\beta}(x)$$

$$\frac{n(x)}{a_{0}} = \psi^{\dagger}_{R\alpha}\psi_{R\beta} + \psi^{\dagger}_{L\alpha}\psi_{L\beta} + (-1)^{x/a_{0}}(\psi^{\dagger}_{R\alpha}\psi_{L\beta} + \psi^{\dagger}_{L\alpha}\psi_{R\beta})$$

$$\frac{n(x)}{a_{0}} = (\mathcal{J}^{0} + \overline{\mathcal{J}}^{0}) + (-1)^{x/a_{0}}tr\left[(\Phi^{\frac{1}{2}} + \Phi^{(\frac{1}{2})\dagger})\right]$$
(36)

$$\mathbf{S}(x) = c_{\alpha}^{\dagger}(x)\frac{\sigma_{\alpha\beta}}{2}c_{\beta}(x)$$

$$\frac{\mathbf{S}^{a}(x)}{a_{0}} = \psi_{R\alpha}^{\dagger}\frac{\sigma_{\alpha\beta}^{a}}{2}\psi_{R\beta} + \psi_{L\alpha}^{\dagger}\frac{\sigma_{\alpha\beta}^{a}}{2}\psi_{L\beta} + (-1)^{x/a_{0}}(\psi_{R\alpha}^{\dagger}\frac{\sigma_{\alpha\beta}^{a}}{2}\psi_{L\beta} + \psi_{L\alpha}^{\dagger}\frac{\sigma_{\alpha\beta}^{a}}{2}\psi_{R\beta})$$

$$\frac{\mathbf{S}^{a}(x)}{a_{0}} = (\mathcal{J}^{a} + \overline{\mathcal{J}}^{a}) + (-1)^{x/a_{0}}tr\left[\sigma^{a}/2(\Phi^{\frac{1}{2}} + \Phi^{(\frac{1}{2})\dagger})\right].$$
(37)

The factor  $(-1)^{x/a_0}$  alternates from one site to the next. The first term of Eq. (37) constitute the local magnetization and the last term is the local staggered magnetization. This formula actually allows an exact determination of spin correlation function. A detailed calculation can be found in appendix B.

Having discussed the free theory, we now turn to the interaction case and we restrict ourselves here exclusively to to spin-1/2 chains case. We first observed that the interaction density of Hubbard's Hamiltonian is given by

$$\frac{1}{a_0}Un_{\uparrow}n_{\downarrow} = a_0U(\frac{1}{4}n^2 - \frac{1}{3}\mathbf{S}^2).$$
(38)

This formula may obtained using the following identities

$$\sigma_{ij}^{a}\sigma_{kl}^{a} = 2\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl} 
\mathbf{S}^{2} = (3/4) - (3/2)(n_{\uparrow}n_{\downarrow}) 
n^{2} = n - 2(n_{\uparrow}n_{\downarrow}).$$
(39)

This rewriting of the interaction permits to express it in terms of rotation invariant quantities. From (36) and (37), the following identities can be derived

$$n^{2} = \left[ \mathcal{J}^{0} \mathcal{J}^{0} + \overline{\mathcal{J}}^{0} \overline{\mathcal{J}}^{0} + \mathcal{J}^{0} \overline{\mathcal{J}}^{0} - 4 \mathcal{J}^{a} \overline{\mathcal{J}}^{a} \right] - \frac{1}{3} (\mathcal{J}^{0} + \overline{\mathcal{J}}^{0}) - \frac{1}{2} \left[ \psi^{\dagger}_{R\alpha} \psi_{L\alpha} \psi^{\dagger}_{R\beta} \psi_{L\beta} + H.c. \right] \mathbf{S}^{2} = \left[ \mathcal{J}^{a} \mathcal{J}^{a} + \overline{\mathcal{J}}^{a} \overline{\mathcal{J}}^{a} + 3 \mathcal{J}^{a} \overline{\mathcal{J}}^{a} - \frac{3}{4} \mathcal{J}^{0} \overline{\mathcal{J}}^{0} \right] - \frac{1}{4} (\mathcal{J}^{0} + \overline{\mathcal{J}}^{0}) - \frac{3}{16} \left[ \psi^{\dagger}_{R\alpha} \psi_{L\alpha} \psi^{\dagger}_{R\beta} \psi_{L\beta} + H.c. \right]$$
(40)

Where we have used the currents SU(2) and U(1) represented in (31) and (34). These expressions are correct only at half-filling: we have used the fact that  $e^{\pm 4ik_F} = 1$ . In the total, the density of interaction is

$$\frac{Un_{\uparrow}n_{\downarrow}}{a_{0}} = \lambda_{1}(\mathcal{J}^{0}\mathcal{J}^{0} + \overline{\mathcal{J}}^{0}\overline{\mathcal{J}}^{0}) + \lambda_{2}(\mathcal{J}^{a}\mathcal{J}^{a} + \overline{\mathcal{J}}^{a}\overline{\mathcal{J}}^{a}) + \lambda_{3}\mathcal{J}^{0}\overline{\mathcal{J}}^{0} + \lambda_{4}\mathcal{J}^{a}\overline{\mathcal{J}}^{a} + \lambda_{5}\left[\psi_{R\alpha}^{\dagger}\psi_{L\alpha}\psi_{R\beta}^{\dagger}\psi_{L\beta} + H.c.\right].$$
(41)

By setting,  $A = a_0 U$ , then we can write

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 $\lambda_1 = \frac{1}{4}A$   $\lambda_2 = -\frac{1}{3}A$   $\lambda_3 = \frac{1}{2}A$   $\lambda_4 = -2A\lambda_5 = -\frac{1}{16}A$ 

# 4 Spin-charge separation

The translation of the interaction in terms of bosons is immediate since it is naturally expressed in terms of currents  $\mathcal{J}^0$  and  $\mathcal{J}^a$ . The only term, which has not been translated explicitly until now, is the last term of Eq. (41). However, according to the formula

$$\left[\psi_{R\alpha}^{\dagger}\psi_{L\alpha}\psi_{R\beta}^{\dagger}\psi_{L\beta} + H.c.\right] = \left[g_{\alpha\beta}g_{\beta\alpha} + H.c\right].$$
(42)

This term corresponds to the spin 1 affine primary  $\Phi^{(1)}$  with conformal dimensions  $h = \bar{h} = 1/(S+1)$ , so we can write

$$[g_{\alpha\beta}g_{\beta\alpha} + H.c] \equiv tr\Phi^{(1)},\tag{43}$$

and hence it does not contain any SU(2) degrees of freedom but U(1) degree of freedom. Thus, the SU(2) excitations are independent of the U(1) degree of freedom: there is a complete separation of the dynamics of the spin and charge degrees of freedom. Indeed, the interaction terms have separated completely in two groups: the charge terms ( $\lambda_1$ ,  $\lambda_3$  and  $\lambda_5$ ) and spin terms ( $\lambda_2$ and  $\lambda_4$ ). The Lagrangian (41) is not difficult to study. The simplest information we may extract from it is the scaling dimension of the various perturbations. Thus, there is a marginal operator for all k, namely  $\mathcal{J}^a \overline{\mathcal{J}}^a$  (which is a primary field with respect to the Virasoro algebra). Current operator  $\mathcal{J}^a$  has the conformal weight  $(h; \bar{h}) = (1, 0)$  and  $\overline{\mathcal{J}}^a$  has the conformal weight  $(h; \bar{h}) = (1, 0)$ . Thus the  $\mathcal{J}^a \overline{\mathcal{J}}^a$  operator has the conformal weight  $(h; \bar{h}) = (1, 1)$  which has the scaling dimension  $\Delta = h + \bar{h} = 2$  and the conformal spin 0. As a consequence, the fourth term is marginally irrelevant and gives the well-known logarithmic corrections to correlators [18]. Moreover, the third term in (41) is "killed" by a redefinition of the U(1) gauge field  $a\mu$  (cf. Appendix A). In addition, affine (Kac-Moody) selection rules forbid the appearance of the relevant operator  $\Phi^{(1)}$ , since we treat the s = 1/2 case. Thus we have to deal with the first and second term in right hand side of Eq. (41). The latters coincide respectively with the energy-momentum tensor of the massless free boson model and of the WZW model. Remember that the energy-momentum tensor for the WZW model is constructed from the Kac-Moody currents according to the Sugawara construction [19]. We then have an effective massless theory in accordance with Haldane's predictions.

Let us now turn our attention to the system

$$H_{\text{Heisenberg}} = J \sum_{i} \mathbf{S}_{i} \cdot \mathbf{S}_{i+1} + K \sum_{i} \mathbf{S}_{i} \cdot \mathbf{S}_{i+2}.$$

In the limit  $J \ll K$ , one may view the system as a pair of interwoven, antiferromagnetic chains with a small interchain interaction J. Each chain could be described by the level-1 WZW model. Therefore, in that regime and in the continuum limit, the system may be regarded as two level-1 WZW models, plus some perturbations. Let  $\mathcal{J}^a$  and  $\overline{\mathcal{J}}^a$  denote the SU(2) currents on one chain and  $\mathcal{J}'^a$  and  $\overline{\mathcal{J}}'^a$  the corresponding currents on the other chain The first perturbation is marginally irrelevant and given by two copies of the fourth term (Eq. (41))

$$\mathcal{L}' = \alpha (\mathcal{J}^a \overline{\mathcal{J}}^a + \mathcal{J}'^a \overline{\mathcal{J}}'^a), \tag{44}$$

where  $\alpha \sim U/|t|$ . The second perturbation is the interchain interaction (J). In the continuum limit and using Eq. (37), it can be shown without difficulty to be

$$\mathcal{L} = \beta (\mathcal{J}^a + \overline{\mathcal{J}}^a) (\mathcal{J}'^a + \overline{\mathcal{J}}'^a), \tag{45}$$

where  $\beta$  is small and proportional to the interchain coupling J. The relevance or irrelevance of a perturbation is determined, as a first approximation, from the scaling dimensions of the various fields at the WZW fixed point. A perturbation of the form  $\mathcal{J}^a \overline{\mathcal{J}}^a$  is marginal as explained above, while a perturbation of the form  $\mathcal{J}^a \mathcal{J}^a$  violates Lorentz (or rotation) invariance. Discarding non-Lorentz invariant terms, which do not contribute to the one-loop renormalization group equations, one can conclude that the system (2) is equivalent to two level-1 WZW models. We thus have a free-field description of the system (2). Notice that two coupled level-1 WZW models are equivalent to one level-2 WZW model, plus one Ising model or real fermion (i.e.  $WZW_{k=1} \otimes WZW_{k=1} \equiv WZW_{k=2} \otimes Ising$ ). The SU(2) WZW model at level k = 2, contains two scaling fields : a spin doublet  $g_{mn}$   $(m, n \in \{-\frac{1}{2}, \frac{1}{2}\})$  with left and right conformal dimensions  $\{\frac{3}{16}, \frac{3}{16}\}$  and a spin triplet  $\Phi_{mn}(m, n \in \{-1, 0, 1\})$  with dimensions  $(\frac{1}{2}, \frac{1}{2})$ . They are respectively  $2 \times 2$  and  $3 \times 3$  matrix fields. In addition, as long as K and J are not too different, one may assume short range AF order along and accross the chains, and work out a direct mapping with the NL $\sigma$ M. For spin-1/2 chains this analysis is complicated by the existence of topological term. We will back to these issues in next publication.

# 5 Conclusion

In this paper, we have shown that the long distance magnetic behaviour of 1D (AF) chain is given by the NL $\sigma$ M. Moreover, when taking the continuum limit "à la Affleck": one tends conjointly the step  $a_0$  and the quantum number s to zero and infinity respectively while maintaining constant measurable physical entities c and  $g^2$ , the velocity of the magnons and the coupling constant, there appears in the Lagrangian an additional term, the topological term characterizing the statistics of excitations. More precisely, we sought by mean of Liouville theorem, an effective field theory that includes naturally a topological term. Haldane conjecture has been recovered using group theoretical methods and Non-abelian bosonization technique. We have also seen that the level-1 SU(2) WZW model with a certain marginally irrelevant perturbation describes the low-energy phenomena of Heisenberg model with spin-1/2. Likewise, in the conformal limit, the so-called Heisenberg ladder is equivalent to two level-1 WZW models. Finally, let us point out that the close interplay between geometry, topology and algebra turned out to be a most crucial point in the analysis of low dimensional field theories and allows one to push forward our understanding of spin chains much further.

# 6 Appendix A: $SU(N)_1$ WZW theory as a fermion coset

It is known that the  $SU(N)_1$  CFT can be formulated as a constrained fermionic model, that is as a U(N)/U(1) fermionic coset theory [17]. The constraint is imposed on a system of N free Dirac fermions by requiring that physical states  $|phys\rangle$  are singlet under the U(1) current,

 $\mathcal{J}_n | phys \rangle = 0, \ n \ge 0.$ 

This is achieved in the path integral formulation by introducing a Lagrange multiplier  $a_n$  which acts as a U(1) gauge field with no dynamics. The  $SU(2)_k$  WZW models, can be also represented as fermionic cosets by making use of the general equivalence  $[17]:U(2k)/(U(1) \times SU(k))$ . In this case, in addition to the constraint implemented by the abelian gauge field  $a_n$ , we have to introduce another constraint associated with the SU(k) currents. This constraint will be implemented by a non-abelian gauge field  $B_n$  in the Lie algebra of SU(k), as for example the Lagragian of the fermionic description of the  $SU(2)_1$ WZW model is given by

$$\mathcal{L} = \psi^{\dagger} (\partial + a + B) \psi,$$

this is the coset version of level-1 WZW model.

#### 7 Appendix B: Spin correlation function

This function can be calculated on the basis of the WZW model. In terms of bosons, the spin density is:

$$\mathbf{S}^{a}(x) = (\mathcal{J}^{a} + \overline{\mathcal{J}}^{a}) + (-1)^{x/a_{0}} tr \left[ {}^{2}\sigma^{a}/2(\Phi^{\frac{1}{2}} + \Phi^{(\frac{1}{2})\dagger}) \right],$$
(46)

in the WZW model  $\mathcal{J}^a$  and  $\overline{\mathcal{J}}^a$  are uncorrelated and their self-correlations are given by

$$\langle \mathcal{J}^{a}(x,\tau)\mathcal{J}^{a}(0,0)\rangle \quad \sim \quad \frac{1}{(v\tau - \mathrm{i}x)^{2}} \langle \overline{\mathcal{J}}^{a}(x,\tau)\overline{\mathcal{J}}^{a}(0,0)\rangle \quad \sim \quad \frac{1}{(v\tau + \mathrm{i}x)^{2}}.$$

$$(47)$$

Moreover, we have seen that the low-temperature behavior of a single Heisenberg chain is described by a Sugawara Hamiltonian with k = 1. The physical particles (pairs of spin-1/2 excitations or spinons), are included through the primary fields  $\Phi^{\frac{1}{2}}$  and  $\Phi^{(\frac{1}{2})\dagger}$  from the representation of the SU(2) group. The  $2k_F$  SDW operator (i.e. the  $2k_F$  spinon density) can be identified

$$N(x) = e^{i2k_F x} tr\sigma \left[ \left( \Phi^{\frac{1}{2}} + \Phi^{\left(\frac{1}{2}\right)\dagger} \right) \right].$$
(48)

and has a scaling dimension 1/2. We immediately deduce that a single spinon at  $k = k_F$  has a scaling dimension 1/4 and behaves as a semion [20]. Exploiting this and the fact that the conformal dimensions of the currents  $\mathcal{J}^a$ ,  $\overline{\mathcal{J}}^a$  are  $(h = 1, \bar{h} = 1)$ , one inevitably finds

$$\begin{split} \langle S^{z}(x,\tau)S^{z}(0,0)\rangle & \backsim \langle \mathcal{J}^{a}(z)\mathcal{J}^{a}(0)\rangle + \langle \overline{\mathcal{J}}^{a}(z)\overline{\mathcal{J}}^{a}(0)\rangle \\ & + (-1)^{x/a_{0}}const. \langle \left[tr\sigma^{a}/2\Phi^{\frac{1}{2}}(z)\right] \left[tr\sigma^{a}/2\Phi^{\frac{1}{2}}(0)\right]\rangle \\ & = A\left[\frac{1}{z^{2}} + \frac{1}{\overline{z}^{2}}\right] + (-1)^{x/a_{0}}\frac{B}{\mid z\mid} (A, B \text{ const.}), \end{split}$$

where

$$z = -i(x - vt) = v\tau - ix; \ \bar{z} = i(x + vt) = v\tau + ix$$
(49)

are the holomorphic (or left) and antiholomorphic (or right) coordinates,  $\tau = it$  is the Euclidian time and v is the characteristic velocity of the model.

Thus we see that the long-range correlation function has two parts: one uniform near (k = 0) and one alternating near  $(k = \pi)$ . The staggered magnetization correlations is therefore decreasing like 1/r, instead of the  $1/r^2$  decay of the uniform correlations. As a consequence, we have temperature dependence of the magnetic susceptibility when taking into account the marginal perturbation  $(\mathcal{J}^a \overline{\mathcal{J}}^a)$  [21], which spoils conformal invariance by inducing logarithmic corrections to the leading scaling behavior.

#### References

- [1] T. Dombre, N. Read, Phys. Rev. B 38 (1988) 7181.
- [2] R. Shankar, N. Read, Nucl. Phys. B 336 (1990).
- [3] J.P. Renard, M. Verdaguer, L.P. Regnault, W.A.G. Erkeles, J. Rossat–Mignod, W.G. Stirling, Europhys. Lett. 3, 945 (1987).
- [4] F. D. M.Haldane, Phys. lett. 93A (1983) 464; Phys. Rev. Lett. 50 (1983)1153.

- [5] L. P. Regnault, I. Zaliznyak, J. P. Renard, and C. Vettier, Phys. Rev. B 50, (1994)9174; A. Zheludev et al., ibid. 53, (1996)15 004; G. Xu et al., ibid. 54, (1996)R6827.
- [6] I. Affleck, Phys. Rev. B 37 (1988) 5186.
- [7] I. Affleck, J. Phys. C 1 (1989) 3047.
- [8] I. Affleck, Nucl. Phys. B 257 (1985) 397.
- [9] A. M. Polyakov, Mod. Phys. lett. A 3 (1988) 325.
- [10] H.A. Bethe, Z. Phys. **71** (1931) 205.
- [11] I. Affleck and F.D.M. Haldane, Phys. Rev. B36, 5291 (1987).
- [12] I. Affleck, in *Fields, Strings and Critical Phenomena, Les Houches, Session XLIX*, edited by E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1988).
- [13] P. W. Anderson, Science 235 (1987) 1196
- [14] F. D. M.Haldane, J. Phys. C, 14 (1981) 2581.
- [15] V. G. Kac, Infinite Dimensional Lie Algebras, Cambridge Univ. Press, Cambridge (1990).
- [16] E. Witten, Commun. Math. Phys. 92, 455 (1984).
- [17] S.G.Naculich and H.J.Schnitzer, Nucl. Phys. B332 (1990) 583.
- [18] I. Affleck, D. Gepner, H. J. Schulz, and T. Ziman, J. Phys. A 22 511 (1989)
- [19] H. Sugawara, A field theory of currents, Phys. Rev. 170 (1968)1659.
- [20] P. Bouwknegt and K. Schoutens, Phys. Rev. lett. 82, (1999)2757.
- [21] S. Eggert, I. Affleck, and M. Takahashi, preprint, cond-mat/9404062