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Field theories for frustrated antiferromagnetic spin chains

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Abstract. We study the antiferromagnetic spin chain with both dimerization and frustration. The classical ground state has three phases, a Néel phase, a spiral phase and a collinear phase, which we study through a nonlinear sigma-model approach. In the spiral phase, the field theory becomes $SO(3) \times SO(3)$ and Lorentz invariant at long distances, a model which is exactly solvable. The low-energy spectrum is doubly degenerate with massive 'elementary' spin-1/2 particles and 'two-particle' triplet and singlet physical excitations. The field theory also supports Z_2 solitons which lead to a double degeneracy of the ground state for half-integer spins (when there is no dimerization).

Antiferromagnets in low dimensions have been extensively studied in recent years, partly because of their possible relevance to high- T_c superconductors and partly due to the variety of theoretical tools which have become available. The latter include nonlinear sigma-model (NLSM) field theories [1–6], Schwinger boson mean-field theories [7], exact diagonalization of small systems [8], and the density matrix renormalization group (DMRG) method [9–13]. In one dimension, NLSM theories in particular have received special attention ever since Haldane [1] conjectured that integer-spin models would have a gap (unlike half-integer-spin chains), and this prediction was verified experimentally for the compound NENP [14].

In this paper, we study a general Heisenberg spin chain with both dimerization (an alternation δ of the nearest-neighbour (nn) couplings) and frustration (a next-nearest-neighbour (nnn) coupling J_2). Even classically (i.e. as the spin $S \to \infty$), we find that the system has a rich ground-state 'phase diagram', with three distinct phases, a Néel phase, a spiral phase and a collinear phase (defined below) [15]. For large but finite S, long-wavelength fluctuations about the classical ground state can be described by nonlinear field theories. These field theories are explicitly known in the Néel phase [1, 2] and in the spiral phase (for $\delta = 0$) [5, 6]. Here we also present the theory for the collinear phase (explicitly for $\delta = 1$, although we argue that the qualitative features persist for $\delta \neq 1$). While the Néel phase has been extensively studied, various aspects like the ground-state degeneracy and the low-energy spectrum are not well understood either in the spiral or collinear phases.

We first recapitulate the results of the field theory and the renormalization group (RG) analysis in the Néel and spiral phases. For the spiral phase, we use a (previously derived) one-loop β -function to show that the field theory for an arbitrary J_1-J_2 model flows to an SO(3) × SO(3)-symmetric and Lorentz invariant theory with an analytically known spectrum [16]. We *predict* that the low-energy excitations of integer-spin chains in the

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spiral phase should be doubly degenerate triplets and singlets. We compare the predicted spectrum with the numerically known spectra for the S = 1 and S = 1/2 models. We also discuss how the presence of Z_2 solitons (supported by the field theory) affects the ground-state degeneracy for integer and half-integer spins.



Figure 1. A classical phase diagram of the $J_1-J_2-\delta$ spin chain.

The Hamiltonian for the frustrated and dimerized spin chain is given by

$$H = J_1 \sum_{i} (1 + (-1)^i \delta) \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + J_2 \sum_{i} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}$$
(1)

where $S_i^2 = S(S+1)\hbar^2$, the couplings $J_1, J_2 \ge 0$, and δ lies between 0 and 1. Classically (for $S \to \infty$), the ground state is a coplanar configuration of the spins with energy per spin equal to

$$E_0 = S^2 \left[\frac{J_1}{2} (1+\delta) \cos \theta_1 + \frac{J_1}{2} (1-\delta) \cos \theta_2 + J_2 \cos(\theta_1 + \theta_2) \right]$$
(2)

where θ_1 is the angle between the spins S_{2i} and S_{2i+1} and θ_2 is the angle between S_{2i} and S_{2i-1} . Minimization of the classical energy with respect to the θ_i yields the following phases.

(i) Néel: this phase has $\theta_1 = \theta_2 = \pi$ and is stable for $1 - \delta^2 > 4J_2/J_1$.

(ii) Spiral: here, the angles θ_1 and θ_2 are given by the upper and lower signs respectively in

$$\cos \theta_{i} = -\frac{1}{1 \pm \delta} \left[\frac{1 - \delta^{2}}{4J_{2}/J_{1}} \pm \frac{\delta}{1 - \delta^{2}} \frac{4J_{2}}{J_{1}} \right]$$
(3)

where $\pi/2 < \theta_1 < \pi$ and $0 < \theta_2 < \pi$. This phase is stable for $1 - \delta^2 < 4J_2/J_1 < (1 - \delta^2)/\delta$. (iii) Collinear: this phase (which needs both dimerization and frustration) is defined to have $\theta_1 = \pi$ and $\theta_2 = 0$. It is stable for $(1 - \delta^2)/\delta < 4J_2/J_1$.

These three phases are depicted in figure 1.

We now study the spin-wave spectrum around the classical ground state [17]. A detailed analysis will be presented elsewhere [18]. In the Néel phase, we recover the well known result that there are two gapless modes with equal velocities. In the spiral phase, we find three modes, two with the same velocity describing out-of-plane fluctuations and one with a higher velocity describing in-plane fluctuations. In the collinear phase, we get two gapless modes with equal velocities just as in the Néel phase. The three phases also differ in the behaviour of the spin-spin correlation function S(q) in the classical limit. S(q) is peaked at $q = \pi$ in the Néel phase, for $\pi/2 < q < \pi$ in the spiral phase and at $q = \pi/2$ in the collinear phase. Even for S = 1/2 and 1, DMRG studies have seen this feature of S(q) in the Néel and spiral phases [10]. The collinear phase has been observed numerically in reference [11], which refers to it as the $\uparrow\uparrow\downarrow\downarrow$ phase.



Figure 2. A plot of $\ln(\zeta/a)/S$ versus J_2/J_1 for $\delta = 0$.

To study nonperturbative aspects, the NLSM approach is convenient since the RG can be used to improve naive perturbation results. The NLSM is well known in the Néel phase [1, 2]. It is a scalar field theory with $c = 2J_1aS\sqrt{1-\delta^2-4J_2/J_1}$ as the spinwave velocity, $g^2 = 2/S\sqrt{1-\delta^2-4J_2/J_1}$ as the coupling constant and a topological term. This field theory is gapless for $\theta = \pi \mod 2\pi$ (where $\theta = 2\pi S(1-\delta)$ is the coefficient of the topological term), with the correlation function falling off as a power at large separations, and is gapped otherwise. For the gapped theory, the correlations decay exponentially with correlation length ζ , where ζ is found from a one-loop RG calculation to be $\zeta/a = \exp(2\pi/g^2)$. Hence $\ln(\zeta/a) = \pi S\sqrt{1-\delta^2-4J_2/J_1}$. For completeness, this is plotted in figure 2 for $\delta = 0$ and $4J_2/J_1 < 1$.

Recently, the spiral phase has also been studied for $\delta = 0$ [5, 6]. The classical ground state has $\theta_1 = \theta_2 = \theta = \cos^{-1}(-J_1/4J_2)$. The field variable describing fluctuations about the classical ground state is an SO(3) matrix **R**(*x*, *t*) related to the spin variable at the *i*th site as $(S_i)_a = S\mathbf{R}_{ab}\mathbf{n}_b$, where a, b = 1, 2, 3 are the components along the \hat{x} -, \hat{y} - and

 \hat{z} -axes, and n is a unit vector given by

$$n_i = \frac{\hat{x}\cos i\theta + \hat{y}\sin i\theta + a\ell}{|\hat{x}\cos i\theta + \hat{y}\sin i\theta + a\ell|}.$$
(4)

The unit vector n_i describes the orientation of the *i*th spin in the classical ground state and $a\ell$ represents the small deviation from the classical configuration. The resultant Lagrangian density has been derived in reference [6]. It is SO(3)_L × SO(2)_R symmetric and can be parametrized as

$$\mathcal{L} = \frac{1}{2c} \operatorname{tr}(\partial_t \mathbf{R}^{\mathrm{T}} \partial_t \mathbf{R} \, \mathbf{P}_0) - \frac{c}{2} \operatorname{tr}(\partial_x \mathbf{R}^{\mathrm{T}} \partial_x \mathbf{R} \, \mathbf{P}_1)$$
(5)

where

$$c = J_1 Sa(1 + 4J_2/J_1) \sqrt{1 - J_1^2/16J_2^2}$$

and \mathbf{P}_0 and \mathbf{P}_1 are diagonal matrices with entries given by, for \mathbf{P}_0 , $(1/2g_2^2, 1/2g_2^2, 1/g_1^2 - 1/2g_2^2)$ and, for \mathbf{P}_1 , $(1/2g_4^2, 1/2g_4^2, 1/g_3^2 - 1/2g_4^2)$. The couplings g_i are found to be

$$g_{2}^{2} = g_{4}^{2} = \frac{1}{s} \sqrt{\frac{4J_{2} + J_{1}}{4J_{2} - J_{1}}}$$

$$g_{3}^{2} = 2g_{2}^{2}$$

$$g_{1}^{2} = g_{2}^{2}[1 + (1 - J_{1}/2J_{2})^{2}].$$
(6)

Perturbatively, there are three gapless modes, one with velocity cg_2/g_4 and two with velocity cg_1/g_3 . Note that the theory is not Lorentz invariant because $g_1g_4 \neq g_2g_3$. However, the theory is symmetric under SO(3)_L ×SO(2)_R where the SO(3)_L rotations mix the rows of the matrix **R** and the SO(2)_R rotations mix the first two columns. SO(3)_L is the manifestation in the continuum theory of the spin symmetry of the original lattice model. SO(2)_R arises in the field theory because the ground state is planar, and the two out-of-plane modes are identical and can mix under an SO(2) rotation. The Lagrangian is also symmetric under the discrete symmetry parity which transforms **R**(x) \rightarrow **R**(-x)**P** with **P** being the diagonal matrix with entries (-1, 1, -1). An important point to note is that there is no topological term present here (unlike in the NLSM in the Néel phase) and, hence, no apparent distinction between integer and half-integer spins. There is, however, a distinction due to solitons, as we will show later.

At larger distance scales l, the effective couplings $g_i(l)$ evolve according to the β -functions $\beta(g_i) = dg_i/dy$ where $y = \ln(l/a)$. We had earlier computed the one-loop β -functions using the background-field formalism [5]. The β -functions are given by

$$\beta(g_{1}) = \frac{g_{1}^{3}}{8\pi} \left[\frac{g_{1}^{2}g_{3}g_{4}}{g_{2}^{2}} \frac{2}{g_{1}g_{4} + g_{2}g_{3}} + 2g_{1}g_{3} \left(\frac{1}{g_{1}^{2}} - \frac{1}{g_{2}^{2}} \right) \right]$$

$$\beta(g_{2}) = \frac{g_{2}^{3}}{8\pi} \left[g_{1}^{3}g_{3} \left(\frac{2}{g_{1}^{2}} - \frac{1}{g_{2}^{2}} \right)^{2} + 4g_{1}g_{3} \left(\frac{1}{g_{2}^{2}} - \frac{1}{g_{1}^{2}} \right) \right]$$

$$\beta(g_{3}) = \frac{g_{3}^{3}}{8\pi} \left[\frac{g_{3}^{2}g_{1}g_{2}}{g_{4}^{2}} \frac{2}{g_{1}g_{4} + g_{2}g_{3}} + 2g_{1}g_{3} \left(\frac{1}{g_{3}^{2}} - \frac{1}{g_{4}^{2}} \right) \right]$$

$$\beta(g_{4}) = \frac{g_{4}^{3}}{8\pi} \left[g_{3}^{3}g_{1} \left(\frac{2}{g_{3}^{2}} - \frac{1}{g_{4}^{2}} \right)^{2} + 4g_{1}g_{3} \left(\frac{1}{g_{4}^{2}} - \frac{1}{g_{3}^{2}} \right) \right].$$
(7)

We numerically investigate the flow of these couplings using the initial values $g_i(a)$ given in equation (6). These are different from the initial values used in reference [5], where

we had earlier studied the evolution of these equations for the Majumdar–Ghosh model $(J_2 = J_1/2)$ [19]. We find that the couplings flow such that g_1/g_2 and g_3/g_4 approach 1, i.e., the theory flows towards $SO(3)_L \times SO(3)_R$ and Lorentz invariance. Finally, at some length scale ζ , the couplings blow up indicating that the system has become disordered. At the one-loop level, ζ depends on J_2/J_1 but *S* can be scaled out. The situation is, in fact, qualitatively similar to what happens in the Majumdar–Ghosh model.

In figure 2, we show the numerical results for $\ln(\zeta/a)/S$ versus J_2/J_1 for $4J_2/J_1 > 1$. Note that as $4J_2/J_1 \rightarrow 1$ from either side (the Néel phase for integer spin or the spiral phase for any spin), $\ln(\zeta/a) \rightarrow 0$, i.e., the correlation length goes through a minimum. Since $4J_2/J_1 = 1$ separates the Néel and spiral phases, we may call it a disorder point. (For general δ , we have a disorder line $4J_2/J_1 + \delta^2 = 1$ and the correlation length is a minimum on the line separating the two gapped phases.)

The spiral phase is therefore disordered for any spin *S* with a length scale ζ . The theory flows to the principal chiral model with SO(3)_{*L*} × SO(3)_{*R*} and Lorentz invariance at long distances. This model is exactly integrable and its spectrum is analytically known [16]. For all spins *S*, the 'elementary' particle is a massive doublet that transforms according to the spin-1/2 representation of SU(2). The long-wavelength, low-energy physical excitations are 'two-particle' states formed from these elementary particles and are spin-triplet and spin-singlet states[†]. Moreover, as explained in reference [16], these excitations are doubly degenerate. A naive perturbative analysis of the field theory, on the other hand, just reproduces the spin-wave prediction of three modes, two with the same velocity and one with a higher velocity. The power of the field theory approach is precisely this ability to probe the infra-red nonperturbative limit.

Interestingly, the spin-triplet and the spin-singlet excitations and their double degeneracy have actually been seen in numerical studies of the $S = 1 \mod [6, 13]$. This is a remarkable proof of the validity of the field theoretic approach, at least for integer spins. It would be worthwhile to verify the spectrum numerically for other integer spins as well.

DMRG studies [9, 10] of spin-1/2 models, on the other hand, have not seen this double degeneracy in the spectrum, although they also find a triplet to be the lowest-energy excitation over the ground state. However, as we shall explain below, for half-integer spins, the ground state itself is doubly degenerate. Hence the excitations about each of the ground states is only singly degenerate. This feature can also be seen in the exact solution of the Majumdar–Ghosh model [19], although it is not in the spiral phase. The ground state is doubly degenerate and the excitation spectrum consists of a spin triplet and a spin singlet formed from the 'elementary' spin-1/2 solitons [21], in accordance with the field theory solution.

Since the field theory is based on an SO(3)-valued field $\mathbf{R}(x, t)$ and $\pi_1(SO(3)) = Z_2$, it allows Z_2 solitons. The classical field configurations come in two distinct classes with soliton number equal to zero or one. An example of a zero-soliton configuration is given by $\mathbf{R}_0(x, t) = \mathbf{I}$, the identity matrix; this configuration has zero energy and is a classical ground state, A one-soliton configuration is given by

$$\mathbf{R}_{1}(x,t) = \begin{pmatrix} \cos\theta(x) & \sin\theta(x) & 0\\ -\sin\theta(x) & \cos\theta(x) & 0\\ 0 & 0 & 1 \end{pmatrix}$$
(8)

where $\theta(x)$ goes from 0 to 2π as x goes from $-\infty$ to $+\infty$. (For convenience, we choose $\theta(x) = 2\pi - \theta(-x)$.) In terms of spins, this corresponds to progressively rotating the spins

 $[\]dagger$ To apply these conclusions to finite spin chains, it is required that the number of spins N be even, so that periodic boundary conditions can be applied without frustration [20].

so that the spins at the right-hand end of the chain are rotated by 2π with respect to spins at the left-hand end. Since the derivative $\partial_x \theta$ can be made vanishingly small, the difference between the energies of the configurations $\mathbf{R}_0(x, t)$ and $\mathbf{R}_1(x, t)$ can be made arbitrarily small, and one might expect the ground state to be doubly degenerate for infinite system size. To be more explicit, imagine space to be a line running from x = -L/2 to x = L/2, and take $\theta(x) = 2\pi(x + L/2)/L$ in equation (8); thus $\mathbf{R}_1 = \mathbf{I}$ at the end points. Then $\mathbf{R}_1(x, t)$ is a solution of the Euler–Lagrange equations of motion following from equation (5). The energy of this configuration is of order 1/L, and it goes to zero if we let the system size $L \to \infty$.

However, this classical continuum argument needs to be examined carefully in the context of a quantum lattice model. Firstly, do $\mathbf{R}_0(x, t)$ and $\mathbf{R}_1(x, t)$ actually correspond to orthogonal quantum states? For the spin model, if the region of rotation is spread out over an odd number of sites, i.e., if the rotation operator is

$$U = \exp\left(\frac{i\pi}{2m+1} \sum_{n=-m}^{m} (2n+2m+1)S_n^z\right)$$

then $\mathbf{R}_0(x, t)$ and $\mathbf{R}_1(x, t)$ have opposite parities because under parity,

$$S_i^z \to -S_{-i}^z$$
 and $U \to U \exp\left(i 2\pi \sum_{n=-m}^m S_n^z\right)$

Since the sum contains an odd number of spins, the term multiplying U is -1 for half-integer spin and 1 for integer spin. Thus for half-integer spin, $\mathbf{R}_0(x, t)$ and $\mathbf{R}_1(x, t)$ are orthogonal and the argument for double degeneracy of the spectrum is valid. This is just a restatement of the Lieb–Schultz–Mattis theorem [22]. For integer spin, $\mathbf{R}_0(x, t)$ and $\mathbf{R}_1(x, t)$ have the same parity and no conclusion can be drawn regarding the degeneracy of the state.

An alternative argument leading to a similar conclusion can be made following Haldane [23]. We consider a tunnelling process between a zero-soliton configuration $\mathbf{R}_0(x, t)$ and a one-soliton configuration $\mathbf{R}_1(x, t)$. (We choose coplanar configurations for convenience.) Such a tunnelling process is not allowed in the continuum theory (which is why the solitons are topologically stable) because the configurations have to be smooth at all space-time points. But in the lattice theory, discontinuities at the level of the lattice spacing are allowed. In terms of spins, this tunnelling can be brought about by turning each spin $S_i^{(0)}$ in configuration $\mathbf{R}_0(x, t)$ to the spin $S_i^{(1)}$ in configuration $\mathbf{R}_1(x, t)$ by either a clockwise or an anticlockwise rotation. Assuming that the magnitude of the amplitude for the tunnelling is the same (as we will show below), the contribution of the two paths either add or cancel depending on whether the spin is integral or half-integral. This is easily seen through a Berry phase [24] calculation. The difference in Berry phase of the two paths from $S_i^{(0)}$ to $S_i^{(1)}$ is $2\pi S$. Since the soliton involves an odd number of spins, the total Berry phase difference is 0 mod 2π if S is an integer and $\pi \mod 2\pi$ if S is half-integer.

To check that the magnitudes of the amplitudes for tunnelling are the same in the two cases, consider the pair of spins $S_i^{(0)}$ and $S_{-i}^{(0)}$ which need to be rotated to $S_i^{(1)}$ and $S_{-i}^{(1)}$. Since $\theta(x) = 2\pi - \theta(-x)$, the magnitude of the amplitude for the clockwise rotation of $S_i^{(0)}$ to $S_i^{(1)}$ is matched by the magnitude of the amplitude for the anticlockwise rotation of $S_{-i}^{(0)}$ to $S_{-i}^{(1)}$. Hence, for the pair of spins taken together, the magnitude of the amplitude for tunnelling is the same for the clockwise and anticlockwise rotations.

Thus, tunnelling between soliton sectors is possible for integer S (thereby breaking the classical degeneracy and leading to a unique quantum ground state) but not for half-integer S (due to cancellations between pairs of paths). This agrees with the earlier Lieb–Schultz–Mattis argument.

Although the NLSM for the spiral phase was explicitly derived only for $\delta = 0$, we expect the same qualitative features to persist when $\delta \neq 0$, because the spin-wave analysis shows that the classical ground state continues to be coplanar and there continue to be three gapless modes (two with identical velocities and the third with a higher velocity [18]). Hence we expect similar RG flows and a similar spectrum. However, the argument for the double degeneracy of the ground state for half-integer spins depends on parity being a good quantum number. When $\delta \neq 0$, the Hamiltonian is not parity invariant and the argument breaks down. This is in agreement with the DMRG studies [10] for periodic chains which show a unique ground state, both for integer and half-integer spins, for $\delta \neq 0$.

At this stage, we would like to point out some limitations of the NLSM studied by us in the spiral phase. Firstly, the NLSM is unable to explain the phenomenon of *spontaneous* dimerization which is known to occur for a spin-1/2 chain with $\delta = 0$ and $J_2/J_1 > 0.241$ [8, 12]. A different nonlinear field theory has been developed recently which is better suited for studying dimerization and also the case $\delta \neq 0$ [25]. Secondly, although the crossover from Néel to spiral (defined by the position of the peak in S(q)) occurs classically at $J_2/J_1 = 1/4$ for $\delta = 0$, the crossover points for small values of spin are rather different, e.g., $J_2/J_1 = 1/2$ for spin-1/2 and 0.373 for spin-1 [13]. This difference is presumably due to corrections of higher order in 1/S which have been ignored in our NLSM. Thirdly, our NLSM does not shed any light on the $Z_2 \times Z_2$ symmetry and its associated string order parameter which are known to play an important role in the spin-1 chain [26, 13]. To conclude, spin chains with small values of *S* exhibit some features which are not anticipated from large-*S* field theories.

Finally, we examine small fluctuations in the collinear phase. The naive expectation is that the field theory would be an O(3) NLSM, analogous to the Néel phase, since the classical ground state is collinear. We can show this explicitly for $\delta = 1$, which is called the Heisenberg ladder case [27, 28]. The field theory here can be obtained in a way similar to the derivation in reference [2] for the Néel phase. For a set of four neighbouring spins, we define

$$\phi(x-a) = \frac{S_{4i} - S_{4i+1}}{2S} \qquad \ell(x-a) = \frac{S_{4i} + S_{4i+1}}{2a}$$

$$\phi(x+a) = \frac{S_{4i+3} - S_{4i+2}}{2S} \qquad \ell(x+a) = \frac{S_{4i+3} + S_{4i+2}}{2a}$$
(9)

where x = (4i+3/2)a is the midpoint of the set of four spins. We then write the Hamiltonian in terms of the fields ϕ and ℓ , Taylor expand to second order in space-time derivatives, and integrate out ℓ to obtain the Lagrangian density

$$\mathcal{L} = \frac{(\partial_t \phi)^2}{2cg^2} - \frac{c(\partial_x \phi)^2}{2g^2} \tag{10}$$

without a topological term. We now find

$$c = 4aS\sqrt{J_2(J_2 + J_1)}$$
 and $g^2 = \frac{1}{S}\sqrt{(J_2 + J_1)/J_2}$

The absence of the topological term means that there is no difference between integer and half-integer spins, and a gap exists in both cases for any finite inter-chain coupling, however small. This is in agreement with numerical work on coupled spin chains [27].

In conclusion, we emphasize that this is the first systematic field theoretic treatment of the general $J_1-J_2-\delta$ model on a chain. Although all experimental spin-chain systems known to date, like NENP and Sr₂CuO₃, are in the Néel phase [14, 29], it would be interesting to find an experimental system with sufficient frustration and dimerization to probe the spiral

and collinear phases. The field theoretic treatment of the spiral phase leads to the prediction of low-energy spin-triplet and spin-singlet excitations, in remarkable agreement with the exact solution of the Majumdar–Ghosh model for S = 1/2 and with numerical solutions of the general frustrated model for S = 1/2 and S = 1. It also leads to the intriguing possibility that the low-energy excitations of integer-spin models may be massive spin-1/2 objects. To actually see these elementary excitations as 'free' particles, a finite external field would have to be applied. It would be interesting to study the model with a finite external field through numerical techniques like DMRG studies or even to look for such excitations experimentally.

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