

# SEMICLASSICAL AND FIELD THEORETIC STUDIES OF HEISENBERG ANTIFERROMAGNETIC CHAINS WITH FRUSTRATION AND DIMERIZATION

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## Abstract

The Heisenberg antiferromagnetic spin chain with both dimerization and frustration is studied. The classical ground state has three phases (a Neel phase, a spiral phase and a colinear phase), around which a planar spin-wave analysis is performed. In each phase, we discuss a non-linear sigma model field theory describing the low energy excitations. A renormalization group analysis of the  $SO(3)$  matrix-valued field theory of the spiral phase leads to the conclusion that the theory becomes  $SO(3) \times SO(3)$  and Lorentz invariant at long distances. This theory is analytically known to have a massive spin-1/2 excitation. We also show that  $Z_2$  solitons in the field theory lead to a double degeneracy in the spectrum for half-integer spins.

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## I. INTRODUCTION

Antiferromagnets in low dimensions have continued to draw considerable interest in recent years, mainly because of their possible relevance to high  $T_c$  superconductors. A large variety of theoretical tools have become available to study them including non-linear sigma model (NLSM) field theories [1-6], Schwinger boson [7] and other bosonic mean field theories [8], fermionic mean field theories [9], series expansions [10], exact diagonalization of small systems [11], and the density matrix renormalization group (DMRG) method [12, 13]. In particular, one of the most useful tools has been the use of the non-linear sigma model (NLSM) field theories [1-6]. These theories display interesting features such as dynamical mass generation and existence of topological soliton solutions, which are of relevance in spin models. In fact, it was the mapping of the  $O(3)$  NLSM to the Heisenberg antiferromagnet which led Haldane [1] to his celebrated conjecture that integer spin models would have a gap, contrary to the known solution for the spin-1/2 model. The experimental verification [14] of this conjecture has given special impetus to the study of NLSM field theories for spin models. Ever since then, various generalizations of the Heisenberg antiferromagnetic spin chain including models with dimerization and/or frustration [15] and coupled chains or Heisenberg ladders [16] have been studied.

In this paper, we study a general Heisenberg spin chain with both dimerization (an alternation  $\delta$  of the nearest neighbor (nn) couplings) and frustration (a next-nearest neighbor (nnn) coupling  $J_2$ ). Even in the classical spin  $S \rightarrow \infty$  limit, the system has a rich ground state ‘phase diagram’, [17] with three distinct phases, a Neel phase, a spiral phase and a colinear phase (defined below). For large, but finite  $S$ , a spin-wave analysis *a la* Villain [18] can be performed which gives the spectrum of low energy excitations about the classical ground state. This is described in Sec. II.

The Neel phase via the Haldane mapping to an  $O(3)$  NLSM is well-known to be gapless for half-integer spins but gapped for integer spins [1, 2]. An interesting and important question to address is whether this distinction persists in the spiral and colinear phases as well. To answer this, we need to describe the long wavelength fluctuations about the classical ground state in these phases as well by non-linear field theories which are capable of systematic improvement by renormalization group techniques. This has been identified in the spiral phase (for  $\delta = 0$ ) [5, 6], and in the colinear phase for

$\delta = 1$ , which corresponds to two coupled spin chains [15, 16]. However, while the Neel phase has been extensively studied, various aspects like the ground state degeneracy and the low energy spectrum are not well understood in the spiral and colinear phases.

For completeness and to set the notation, we first review in Sec. III A, the NLSM and the RG in the Neel phase for arbitrary  $J_2$  and  $\delta$ . For the spiral phase, in Sec. III B, we obtain the  $SO(3)$ -valued non-linear field theory and show using a (previously derived) one-loop  $\beta$ -function that the field theory flows to an  $SO(3) \times SO(3)$  symmetric and Lorentz invariant theory with an analytically known spectrum [19]. However, this does not directly lead to a distinction between integer and half-integer spins. But in Sec. III C, we discuss how the presence of  $Z_2$  solitons affects the ground state degeneracy and the low energy spectrum and does provide a distinction. We are led to the conclusion that the system is gapped both for integer and non-integer spins, but the ground state is degenerate for half-integer spins (when there is no dimerization). In Sec. III D, we briefly discuss the NLSM for a spin ladder. It is qualitatively similar to the one in the Neel phase. However, no topological term is induced and there is no distinction between the integer and half-integer spin cases. A shorter version of these results will appear elsewhere [15]. Finally, we make some concluding remarks in Sec. IV.

## II. CLASSICAL PHASE DIAGRAM AND SPIN WAVE ANALYSIS

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

$$H = J_1 \sum_i (1 + (-1)^i \delta) \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}, \quad (1)$$

where  $\mathbf{S}_i^2 = S(S+1)\hbar^2$ , the coupling constants  $J_1, J_2 \geq 0$  and the dimerization parameter  $\delta$  lies between 0 and 1. (We will henceforth set  $\hbar = 1$ ). Classically (for  $S \rightarrow \infty$ ), the ground state is a coplanar configuration of the spins with energy per spin equal to

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

where  $\theta_1$  is the angle between the spins  $\mathbf{S}_{2i}$  and  $\mathbf{S}_{2i+1}$  and  $\theta_2$  is the angle between the spins  $\mathbf{S}_{2i}$  and  $\mathbf{S}_{2i-1}$ . Minimization of the classical energy with respect to the  $\theta_i$  yields the following phases.

- (i) Neel: This phase has  $\theta_1 = \theta_2 = \pi$  and is stable for  $1 - \delta^2 > 4J_2/J_1$ .  
(ii) Spiral: Here, the angles  $\theta_1$  and  $\theta_2$  are given by

$$\begin{aligned} \cos \theta_1 &= -\frac{1}{1+\delta} \left[ \frac{1-\delta^2}{4J_2/J_1} + \frac{\delta}{1+\delta^2} \frac{4J_2}{J_1} \right] \\ \text{and } \cos \theta_2 &= -\frac{1}{1-\delta} \left[ \frac{1-\delta^2}{4J_2/J_1} - \frac{\delta}{1-\delta^2} \frac{4J_2}{J_1} \right], \end{aligned} \quad (3)$$

where  $\pi/2 < \theta_1 < \pi$  and  $0 < \theta_2 < \theta_1$ . This phase is stable for  $1 - \delta^2 < 4J_2/J_1 < (1 - \delta^2)/\delta$ .

- (iii) Colinear: 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 phases along with the phase boundaries are depicted in Fig. 1.

We now study the spin wave spectrum about the ground state. Before describing the details of the calculations, we state the main results. In the Neel phase, we find two zero modes with equal velocities. In the spiral phase, we have three modes, two with the same velocity describing out-of-plane fluctuations and one with a higher velocity describing in-plane fluctuations. In the colinear phase, we get two zero modes with equal velocities just as in the Neel phase. The three phases also differ in the behavior of the spin-spin correlation function  $S(q) = \sum_n \langle \vec{S}_o \cdot \vec{S}_n \rangle \exp(-iqn)$  in the classical limit.  $S(q)$  is peaked at  $q = (\theta_1 + \theta_2)/2$ , *i.e.*, at  $q = \pi$  in the Neel phase, at  $\pi/2 < q < \pi$  in the spiral phase and at  $q = \pi/2$  in the colinear phase. Even for  $S = 1/2$  and 1, DMRG studies have seen this feature of  $S(q)$  in the Neel and spiral phases [13]. The colinear region has not yet been probed numerically.

Since the classical ground state is coplanar (with the spins lying in, say, the  $\hat{\mathbf{x}} - \hat{\mathbf{y}}$  plane) in all the phases, it is more convenient to develop the spin wave theory by parametrizing the spin operators in terms of Villain's variables [18], rather than the usual Holstein-Primakoff variables [20]. The spin variables at each site are expressed in terms of two conjugate variables  $S_{iz}$  and  $\phi_i$  as

$$\begin{aligned} S_i^+ &= \exp(i\phi_i) \left[ \left(S + \frac{1}{2}\right)^2 - \left(S_{iz} + \frac{1}{2}\right)^2 \right]^{1/2}, \\ S_i^- &= \left[ \left(S + \frac{1}{2}\right)^2 - \left(S_{iz} + \frac{1}{2}\right)^2 \right]^{1/2} \exp(-i\phi_i), \\ \text{and } S_i^z &= \frac{1}{i} \frac{\partial}{\partial \phi_i}. \end{aligned} \quad (4)$$

The periodic operator  $\phi_i$  (with  $\phi_i \equiv \phi_i + 2\pi$ ) satisfies the commutation relation

$$\left[ \phi_i, \frac{S_{jz}}{S} \right] = \frac{i}{S} \delta_{ij}. \quad (5)$$

In the large- $S$  limit, the discreteness of  $S_{iz}/S$  and the periodicity of  $\phi_i$  can be ignored.  $S_{iz}$  and  $\phi_i$  can then be thought of as canonically conjugate and continuous momentum and position operators. In the classical limit  $S \rightarrow \infty$ ,  $S_{iz}/S \rightarrow 0$  and  $\phi_i$  is fixed at a value  $\bar{\phi}_i$  which is the angle made by the classical spin  $\mathbf{S}_i$  relative to the  $\mathbf{x}$ -axis in the plane.

We now expand the square roots in Eq. (4) and keep terms only up to order  $1/S$ . On expanding the angles  $\phi_i$  to quadratic order about  $\bar{\phi}_i$ , we obtain

$$\begin{aligned} S_i^+ &= \exp(i\bar{\phi}_i) \left(S + \frac{1}{2}\right) \left(1 + i\sigma_i - \frac{1}{2}\sigma_i^2\right) \left(1 - \frac{1}{2} \frac{(S_{iz} + \frac{1}{2})^2}{(S + \frac{1}{2})^2}\right), \\ S_i^- &= \exp(-i\bar{\phi}_i) \left(S + \frac{1}{2}\right) \left(1 - i\sigma_i - \frac{1}{2}\sigma_i^2\right) \left(1 - \frac{1}{2} \frac{(S_{iz} + \frac{1}{2})^2}{(S + \frac{1}{2})^2}\right), \end{aligned} \quad (6)$$

where  $\sigma_i$  describes in-plane fluctuations (about the angle  $\bar{\phi}_i$ ) and  $S_{iz}/S$  describes out-of-plane fluctuations. In the presence of dimerization  $\delta$ , the unit cell contains 2 sites and has size  $2a$ , where  $a$  is the lattice spacing. We therefore define

$$\begin{aligned} S_n^{(1)} &= S_{2n+1,z}, & S_n^{(2)} &= S_{2n,z}, \\ \text{and } \sigma_n^{(1)} &= \sigma_{2n+1}, & \sigma_n^{(2)} &= \sigma_{2n}. \end{aligned} \quad (7)$$

and their Fourier components

$$\begin{aligned} S_k^{(a)} &= \sqrt{\frac{2}{N}} \sum_n S_n^{(a)} \exp(-i2kna), \\ \text{and } \sigma_k^{(a)} &= \sqrt{\frac{2}{N}} \sum_n \sigma_n^{(a)} \exp(-i2kna), \end{aligned} \quad (8)$$

where  $a = 1, 2$ , and

$$[\sigma_k^{(a)}, S_{k'}^{(b)}] = i\delta^{ab}\delta_{k+k',0} \quad (9)$$

for the doubled unit cell. Substituting (6) in terms of the Fourier components of the doubled unit cell in (1), we find

$$H = E_o + \sum_k \sum_{a,b} \left[ S_k^{(a)} \underline{A}_k^{ab} S_{-k}^{(b)} + S^2 \sigma_k^{(a)} \underline{B}_k^{ab} \sigma_{-k}^{(b)} \right], \quad (10)$$

where  $0 < k < \pi/2a$  and  $a, b = 1, 2$ ; and  $\underline{A}_k$  and  $\underline{B}_k$  are  $2 \times 2$  hermitian matrices of the form

$$\begin{aligned} \underline{A}_k &= \begin{pmatrix} a_1 & a_2 + a_3 e^{i2ka} \\ a_2 + a_3 e^{-i2ka} & a_1 \end{pmatrix}, \\ \text{with } a_1 &= -J_1 [(1 + \delta) \cos \theta_1 + (1 - \delta) \cos \theta_2] \\ &\quad - 2J_2 \cos(\theta_1 + \theta_2) + 2J_2 \cos 2ka, \\ a_2 &= J_1 (1 + \delta), \quad a_3 = J_1 (1 - \delta), \end{aligned} \quad (11)$$

and

$$\begin{aligned} \underline{B}_k &= \begin{pmatrix} b_1 & b_2 + b_3 e^{i2ka} \\ b_2 + b_3 e^{-i2ka} & b_1 \end{pmatrix}, \\ \text{with } b_1 &= -J_1 [(1 + \delta) \cos \theta_1 + (1 - \delta) \cos \theta_2] \\ &\quad - 2J_2 \cos(\theta_1 + \theta_2) + 2J_2 \cos(\theta_1 + \theta_2) \cos 2ka, \\ b_2 &= J_1 (1 + \delta) \cos \theta_1, \quad b_3 = J_1 (1 - \delta) \cos \theta_2. \end{aligned} \quad (12)$$

These formulae hold for all three phases; the angles  $\theta_i$  were given earlier for each phase. To find the spin wave spectrum  $\omega(k)$ , we have to diagonalize  $\underline{A}_k$  and  $\underline{B}_k$ , *i.e.*, we have to find a matrix  $U$  (not necessarily unitary) such that  $\det U = 1$ , and  $UA_k U^\dagger$  and  $U^{-1\dagger} B_k U^{-1}$  are real diagonal matrices with entries  $\text{diag}(\alpha_1, \alpha_2)$  and  $\text{diag}(\beta_1, \beta_2)$  respectively. Then the energies of modes of momentum  $k$  are given by  $\omega_{1k} = S\sqrt{\alpha_1 \beta_1}$  and  $\omega_{2k} = S\sqrt{\alpha_2 \beta_2}$ . (There are two modes for each  $k$  because a unit cell contains two sites).

In the Neel phase, both the energies vanish at  $k = 0$ . The spin wave velocity  $c$  is defined to be the derivative  $\partial\omega/\partial k$  at the gapless point. We find that  $c = 2J_1 S a \sqrt{1 - \delta^2 - 4J_2/J_1}$  for both branches. In the spiral phase, we find one gapless mode at  $k = 0$  (with a slope  $c_o$ ) and two gapless modes at  $2ka = 2\pi - \theta_1 - \theta_2$ . The latter are counted as two modes because the energy vanishes as one approaches that value of  $k$  both from the left and from the right; and the two slopes  $c_1$  are equal. The expressions for these velocities are quite complicated for general  $\delta$ . (However, we find that the spin wave velocity  $c_o$  is always greater than  $c_1$ ). For  $\delta = 0$ , the expressions simplify to give  $c_o = J_1 S a (1 + 4J_2/J_1) \sqrt{1 - J_1^2/16J_2^2}$  and  $c_1 = c_o \sqrt{[1 + (1 - J_1/2J_2)^2]}/2$ . Finally, in the colinear phase, one of the energies vanishes at  $k = 0$  and the other at  $2ka = \pi$ . The spin wave velocities are equal at the two points and are given by  $c = 2J_1 S a \sqrt{(4J_2\delta/J_1 + \delta^2 - 1)(2J_2/J_1 + \delta + 1)/(2\delta)}$ . One can

also check that in all the cases, the spin wave velocities vanish as we approach the boundary separating any two phases.

The above calculation of the spin wave velocities  $c$  assumes long range order. For finite values of  $S$ , the spin chain models actually have no long range order, *i.e.*, the two-spin correlation function goes to zero at large separation either algebraically or exponentially. However, it is still useful to calculate  $c$  because it is one of the parameters which enters the NLSM field theories; one therefore has a consistency check on the derivation of the field theories.

### III. NLSM FIELD THEORIES

#### A. Neel Phase

To study non-perturbative aspects, the NLSM approach is convenient since the RG can be used to improve naive perturbation results. The NLSM is well-known in the Neel phase [1, 2] and can be most easily derived as follows. The field variable is a unit vector  $\vec{\phi}$ . Since the classical ground state has a periodicity of two sites, we group the spins in two's and define

$$\begin{aligned} \vec{\ell}_{2i+1/2} &= \frac{\mathbf{S}_{2i} + \mathbf{S}_{2i+1}}{2a}, \\ \text{and } \vec{\phi}_{2i+1/2} &= \frac{\mathbf{S}_{2i} - \mathbf{S}_{2i+1}}{2S}. \end{aligned} \quad (13)$$

These variables satisfy the identities

$$\begin{aligned} \vec{\ell} \cdot \vec{\phi} &= 0, \\ \text{and } \vec{\phi}^2 &= 1 + \frac{1}{S} - \frac{a^2 \vec{\ell}^2}{S^2}, \end{aligned} \quad (14)$$

so that  $\vec{\phi}^2 = 1$  in the large- $S$  and long wavelength limit. (We will see below that  $\vec{\ell}$  is proportional to a single space-time derivative of  $\vec{\phi}$ ; hence long wavelength means that  $|a\vec{\ell}| \ll 1$ ). We define the continuum space coordinate  $x = 2ia$  so that  $\delta_{2i,2j}/2a = \delta(x - y)$ . The variables in Eq. (13) therefore satisfy the commutation relations

$$\begin{aligned} [\ell_\alpha(x), \ell_\beta(y)] &= i \epsilon_{\alpha\beta\gamma} \ell_\gamma(x) \delta(x - y), \\ [\ell_\alpha(x), \phi_\beta(y)] &= i \epsilon_{\alpha\beta\gamma} \phi_\gamma(x) \delta(x - y), \\ \text{and } [\phi_\alpha(x), \phi_\beta(y)] &= 0. \end{aligned} \quad (15)$$

where  $\alpha, \beta, \gamma = x, y, z$ , and  $\gamma$  is summed over on the right hand sides. Thus  $\vec{\ell}(x)$  can be identified as the angular momentum of the field  $\vec{\phi}$ , and  $\vec{\ell} = \vec{\phi} \times \vec{\pi}$ , where  $\vec{\pi}$  is the momentum canonically conjugate to  $\vec{\phi}$ . The Hamiltonian (1) can be rewritten in terms of  $\vec{\ell}$  and  $\vec{\phi}$ , and Taylor expanded in space derivatives, *e.g.*,

$$\vec{\phi}_{2i+5/2} = \vec{\phi}_{2i+1/2} + 2a \vec{\phi}'_{2i+1/2} + 2a^2 \vec{\phi}''_{2i+1/2} + \dots \quad (16)$$

For  $\vec{\ell}$ , since it is already proportional to  $\vec{\phi}$ , we only need to keep terms up to  $\vec{\ell}^2$ ,  $\dot{\vec{\ell}}$  and  $\vec{\ell}'$ , where the dot and prime denote time and space derivatives respectively. Finally, we replace the sum  $\sum_{2i} = \int dx/2a$  to obtain a continuum Hamiltonian

$$H = \int dx \left[ \frac{cg^2}{2} \left( \vec{\ell} + \frac{S}{2}(1-\delta)\vec{\phi}' \right)^2 + \frac{c}{2g^2} \vec{\phi}'^2 \right], \quad (17)$$

where  $c$  is the spin wave velocity obtained earlier in the Neel phase, and the coupling constant  $g^2 = 2/(S\sqrt{1-\delta^2-4J_2/J_1})$ . Thus large- $S$  corresponds to weak coupling.

The Hamiltonian in (17) follows from the ‘Lorentz-invariant’ Lagrangian density

$$\mathcal{L} = \frac{\dot{\vec{\phi}}^2}{2cg^2} - \frac{c\vec{\phi}'^2}{2g^2} + \frac{\theta}{4\pi} \vec{\phi} \cdot \dot{\vec{\phi}} \times \vec{\phi}' \quad (18)$$

Here  $c = 2J_1aS\sqrt{1-\delta^2-4J_2/J_1}$  is the spin wave velocity ( $a$  is the lattice spacing) and  $g^2$  is the coupling constant. The third term in (4) is a topological term with  $\theta = 2\pi S(1-\delta)$ . It is known that this field theory is gapless for  $\theta = \pi \bmod 2\pi$  with the correlation function falling off with the power 1 at large separations, and is gapped otherwise [2]. For the gapped theory, the correlations decay exponentially with correlation length  $\zeta$ , where  $\zeta$  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 Fig. 1 for  $\delta = 0$  and  $4J_2/J_1 < 1$ .

## B. Spiral Phase

Recently, the NLSM for the spiral phase has been studied for  $\delta = 0$  [5, 6]. Since the classical ground state is generally not periodic, we will follow the treatment of Ref. [6]. The 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  $\underline{R}(x, t)$  related to the spin variable at the  $i^{\text{th}}$  site as  $(\mathbf{S}_i)_a = S\underline{R}_{ab}\hat{\mathbf{n}}_b$ , where  $a, b = 1, 2, 3$  are the components along the  $\hat{\mathbf{x}}$ ,  $\hat{\mathbf{y}}$  and  $\hat{\mathbf{z}}$  axis, and  $\hat{\mathbf{n}}$  is a unit vector given by

$$\hat{\mathbf{n}}_i = \frac{\hat{\mathbf{x}} \cos i\theta + \hat{\mathbf{y}} \sin i\theta + a\vec{\ell}}{|\hat{\mathbf{x}} \cos i\theta + \hat{\mathbf{y}} \sin i\theta + a\vec{\ell}|}. \quad (19)$$

The unit vector  $\hat{\mathbf{n}}_i$  describes the orientation of the  $i^{\text{th}}$  spin in the classical ground state, and  $a\vec{\ell}$  represents the small deviation from the classical configuration (it is *not* the angular momentum as in our discussion of the Neel phase in (13)). The Hamiltonian in Eq. (1) can be expanded in terms of  $\underline{R}$  and  $\vec{\ell}$ , and Taylor expanded up to second order in space-time derivatives to obtain a continuum Hamiltonian [6]

$$H = \sum_{a,b} \ell_a M_{ab} \ell_b + \text{tr} (\underline{R}'^T \underline{R}' P). \quad (20)$$

Here  $M$  and  $P$  are diagonal matrices with

$$\begin{aligned} M &= \text{diag} (M_{11}, M_{22}, M_{33}) \\ \text{with } M_{33} &= 2J_2 a S^2 (1 + J_1/4J_2)^2, \\ \text{and } M_{11} = M_{22} &= M_{33} [1 + (1 - J_1/2J_2)^2]/4, \end{aligned} \quad (21)$$

and

$$\begin{aligned} P &= \text{diag} (P_{11}, P_{22}, P_{33}) \\ \text{with } P_{11} = P_{22} &= J_2 a S^2 (1 - J_1^2/16J_2^2), \\ \text{and } P_{33} &= 0. \end{aligned} \quad (22)$$

The Lagrangian is then

$$\mathcal{L} = \mathcal{L}_K - H, \quad \text{with } \mathcal{L}_K = aS(\underline{T}\vec{\ell}) \cdot \mathbf{V} \quad (23)$$

where

$$\underline{T} = \text{diag} (1/2, 1/2, 1) \quad \text{and} \quad V_a = -1/2\epsilon_{abc}(\underline{R}^T \dot{\underline{R}})_{bc}. \quad (24)$$

$\mathcal{L}_K$  is obtained by a path integral calculation using spin coherent states [21]. Finally, we integrate out the field  $\vec{\ell}$  which appears quadratically in  $\mathcal{L}$ . The resultant Lagrangian density is found to have an  $SO(3)_L \times SO(2)_R$  symmetry and can be parametrized as

$$\mathcal{L} = \frac{1}{2c} \text{tr}(\partial_t \underline{R}^T \partial_t \underline{R} P_0) - \frac{c}{2} \text{tr}(\partial_x \underline{R}^T \partial_x \underline{R} P_1), \quad (25)$$

where  $c = J_1 S a (1 + 4J_2/J_1) \sqrt{1 - J_1^2/16J_2^2}$ , and  $P_0$  and  $P_1$  are diagonal matrices with entries given by

$$\begin{aligned} P_0 &= \text{diag} \left( \frac{1}{2g_2^2}, \frac{1}{2g_2^2}, \frac{1}{g_1^2} - \frac{1}{2g_2^2} \right) \\ \text{and } P_1 &= \text{diag} \left( \frac{1}{2g_4^2}, \frac{1}{2g_4^2}, \frac{1}{g_3^2} - \frac{1}{2g_4^2} \right). \end{aligned} \quad (26)$$

The couplings  $g_i$  are found to be

$$\begin{aligned} g_2^2 &= g_4^2 = \frac{1}{S} \sqrt{\frac{4J_2 + J_1}{4J_2 - J_1}}, \\ g_3^2 &= 2g_2^2, \\ \text{and } g_1^2 &= g_2^2 [1 + (1 - J_1/2J_2)^2]. \end{aligned} \quad (27)$$

Perturbatively, there are three modes, one gapless mode with the velocity  $cg_2/g_4$  and two gapless modes with the 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  $SO(3)_L \times SO(2)_R$  where the  $SO(3)_L$  rotations mix the rows of the matrix  $\underline{R}$  and the  $SO(2)_R$  rotations mix the first two columns. (To have the full  $SO(3)_L \times SO(3)_R$  symmetry, we need  $g_1 = g_2$  and  $g_3 = g_4$ , *i.e.*, both  $P_0$  and  $P_1$  proportional to the identity matrix.) The  $SO(3)_L$  is the manifestation in the continuum theory of the spin symmetry of the original lattice model. The  $SO(2)_R$  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  $\underline{R}(x) \rightarrow \underline{R}(-x)P$  with  $P$  being the diagonal

matrix (-1,1,-1). An important point to note is that there is no topological term present here (unlike the NLSM in the Neel 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 distances of the order of the lattice spacing  $a$ , the values of the couplings are given in Eq. (27). At larger distance scales  $l$ , the effective couplings  $g_i(l)$  evolve according to the  $\beta$ -functions  $\beta(g_i) = dg_i/dy$  where  $y = \ln(l/a)$ . We have computed the one-loop  $\beta$ -functions using the background field formalism [22]. (Note that since the theory is not Lorentz-invariant, geometric methods cannot be used to obtain the  $\beta$ -functions [4].) The  $\beta$ -functions are given by

$$\begin{aligned}
\beta(g_1) &= \frac{g_1^3}{8\pi} \left[ \frac{g_1^2 g_3 g_4}{g_2^2} \frac{2}{g_1 g_4 + g_2 g_3} + 2g_1 g_3 \left( \frac{1}{g_1^2} - \frac{1}{g_2^2} \right) \right], \\
\beta(g_2) &= \frac{g_2^3}{8\pi} \left[ g_1^3 g_3 \left( \frac{2}{g_1^2} - \frac{1}{g_2^2} \right)^2 + 4g_1 g_3 \left( \frac{1}{g_2^2} - \frac{1}{g_1^2} \right) \right], \\
\beta(g_3) &= \frac{g_3^3}{8\pi} \left[ \frac{g_3^2 g_1 g_2}{g_4^2} \frac{2}{g_1 g_4 + g_2 g_3} + 2g_1 g_3 \left( \frac{1}{g_3^2} - \frac{1}{g_4^2} \right) \right], \\
\text{and } \beta(g_4) &= \frac{g_4^3}{8\pi} \left[ g_3^3 g_1 \left( \frac{2}{g_3^2} - \frac{1}{g_4^2} \right)^2 + 4g_1 g_3 \left( \frac{1}{g_4^2} - \frac{1}{g_3^2} \right) \right]. \quad (28)
\end{aligned}$$

We numerically investigate the flow of these couplings using the initial values  $g_i(a)$  given in Eq.(27). 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  $\zeta$ , the couplings blow up indicating that the system has become disordered. At one-loop,  $\zeta$  depends on  $J_2/J_1$  but  $S$  can be scaled out. In Fig. 2, we show the numerical results for  $\ln(\zeta/a)$  versus  $J_2/J_1$  for  $4J_2/J_1 > 1$ . Note that as  $4J_2/J_1 \rightarrow 1$  from either side (the Neel 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 Neel and spiral phases, we may call it a disorder point. (For general  $\delta$ , we have a disorder line  $4J_2/J_1 + \delta^2 = 1$  and the correlation length is minimum on the disorder line separating the two gapped phases.)

The spiral phase is therefore disordered for any spin  $S$  with a length scale  $\zeta$ . Since the theory flows to the principal chiral model with  $SO(3)_L \times SO(3)_R$  invariance at long distances, we can read off its spectrum from the exact solution given in Ref. [19]. The low energy spectrum consists of a massive

doublet that transforms according to the spin-1/2 representation of  $SU(2)$ . It would be interesting to verify this by numerical studies of the model. DMRG studies [12, 13] of spin-1/2 and spin-1 chains have not seen these elementary excitations so far. It is likely that these excitations are created in pairs and a naive computation of the energy gap would only give the mass of a pair. To see them as individual excitations, it would be necessary to compute the wave function of an excited state and explicitly compute the local spin density as was done in Ref. [23] to study a one magnon state in the Neel phase.

### C. Solitons In The Spiral Phase

Since the field theory is based on an  $SO(3)$ -valued field  $\underline{R}(x, t)$  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. If  $\underline{R}_0(x, t)$  is a zero soliton configuration, then a one soliton configuration is obtained as

$$\underline{R}_1(x, t) = \begin{pmatrix} \cos \theta(x) & \sin \theta(x) & 0 \\ -\sin \theta(x) & \cos \theta(x) & 0 \\ 0 & 0 & 1 \end{pmatrix} \underline{R}_0(x, t), \quad (29)$$

where  $\theta(x)$  goes from 0 to  $2\pi$  as  $x$  goes from  $-\infty$  to  $+\infty$ . (For convenience, we choose  $\theta(x) = 2\pi - \theta(-x)$ , *i.e.*, the twist is parity symmetric about the origin.) In terms of spins, this corresponds to progressively rotating the spins so that the spins at the right end of the chain are rotated by  $2\pi$  with respect to spins at the left end. Since the derivative  $\partial_x \theta$  can be made vanishingly small, the difference in the energies of the configurations  $\underline{R}_0(x, t)$  and  $\underline{R}_1(x, t)$  can be made arbitrarily small, and one might expect to see a double degeneracy in the spectrum.

However, this classical continuum argument needs to be examined carefully in the context of a quantum lattice model. Firstly, do  $\underline{R}_0(x, t)$  and  $\underline{R}_1(x, t)$  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

$$U = \exp\left(\frac{i\pi}{2m+1} \sum_{n=-m}^m (2n+2m+1)S_n^z\right), \quad (30)$$

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

$$S_i^z \rightarrow -S_{-i}^z \quad \text{and} \quad U \rightarrow U \exp(i2\pi \sum_{n=-m}^m S_n^z). \quad (31)$$

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,  $\underline{R}_0(x, t)$  and  $\underline{R}_1(x, t)$  are orthogonal and the argument for double degeneracy of the spectrum is valid. This is just a restatement of the Lieb-Schultz-Mattis theorem [24]. For integer spin,  $\underline{R}_0(x, t)$  and  $\underline{R}_1(x, t)$  have the same parity, and no conclusion can be drawn regarding the degeneracy of the spectrum.

An alternative argument leading to a similar conclusion can be made following Haldane [25]. We consider a tunneling process between a zero soliton configuration  $\underline{R}_0(x, t)$  and a one soliton configuration  $\underline{R}_1(x, t)$ . (We choose coplanar configurations for convenience). Such a tunneling 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 tunneling can be brought about by turning each spin  $\mathbf{S}_i^{(0)}$  in configuration  $\underline{R}_0(x, t)$  to the spin  $\mathbf{S}_i^{(1)}$  in configuration  $\underline{R}_1(x, t)$  by either a clockwise or an anticlockwise rotation. Assuming that the magnitude of the amplitude for the tunneling 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 [21] calculation. The difference in the Berry phase of the two paths from  $\mathbf{S}_i^{(0)}$  to  $\mathbf{S}_i^{(1)}$  is  $2\pi S$ . Since the soliton involves an odd number of spins, the total Berry phase difference is  $0 \bmod 2\pi$  if  $S$  is an integer and  $\pi \bmod 2\pi$  if  $S$  is half-integer.

Now we have to check that the magnitudes of the amplitudes for tunneling are the same in both the cases. To see this, consider the pair of spins  $\mathbf{S}_i^{(0)}$  and  $\mathbf{S}_{-i}^{(0)}$  which need to be rotated to  $\mathbf{S}_i^{(1)}$  and  $\mathbf{S}_{-i}^{(1)}$ . Since  $\theta(x) = 2\pi - \theta(-x)$ , the magnitude of the amplitude for the clockwise rotation of  $\mathbf{S}_i^{(0)}$  to  $\mathbf{S}_i^{(1)}$  is matched by the magnitude of the amplitude for the anticlockwise rotation of  $\mathbf{S}_{-i}^{(0)}$  to  $\mathbf{S}_{-i}^{(1)}$ . Hence, for the pair of spins taken together, the magnitude of the amplitude for tunneling is the same for the clockwise and anticlockwise rotations.

Thus, tunneling 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 model 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 zero modes (two with identical velocities and the third with a higher velocity). 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  $\delta \neq 0$ , parity no longer commutes with the Hamiltonian and the argument breaks down. This is in agreement with the DMRG studies [13] (for periodic chains) which show a unique ground state, both for integer and half-integer spins, for  $\delta \neq 0$ . For open chains, the ground state is sometimes degenerate due to end degrees of freedom. To incorporate such effects, one would have to study NLSM theories on open chains which is beyond the scope of this work.

#### D. Colinear Phase

Finally, we examine small fluctuations in the colinear phase. The naive expectation is that the field theory would be an  $O(3)$  NLSM, analogous to the Neel phase, since the classical ground state is colinear. We can show this explicitly for  $\delta = 1$  which is called the Heisenberg ladder [26]. The field theory in this limit can be derived using the classical periodicity under translation by four lattice sites, similar to the derivation given in Se. IIIA for the Neel phase. For a set of four neighbouring spins, we define

$$\begin{aligned} \vec{\phi}(x-a) &= \frac{\mathbf{S}_{4i} - \mathbf{S}_{4i+1}}{2S}, & \vec{\ell}(x-a) &= \frac{\mathbf{S}_{4i} + \mathbf{S}_{4i+1}}{2a}, \\ \text{and } \vec{\phi}(x+a) &= \frac{\mathbf{S}_{4i+3} - \mathbf{S}_{4i+2}}{2S}, & \vec{\ell}(x+a) &= \frac{\mathbf{S}_{4i+3} + \mathbf{S}_{4i+2}}{2a} \end{aligned} \quad (32)$$

where  $x = (4i + 3/2)a$  is the mid-point of the set of four spins. We then write the Hamiltonian in terms of the fields  $\vec{\phi}$  and  $\vec{\ell}$ , and Taylor expand to second order in space-time derivatives to obtain the Lagrangian (18) *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. In fact, the NLSM predicts a gap for any finite inter-chain coupling, however small. This is in agreement with numerical work on coupled spin chains [26].

#### IV. DISCUSSION

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  $Sr_2CuO_3$ , are in the Neel phase [14, 27], it would be interesting to find an experimental system with sufficient frustration and dimerization to probe the spiral and colinear phases. These phases could also be studied using numerical techniques like DMRG. The field theoretic treatment of the spiral phase leads to the interesting possibility that the low energy excitations of integer spin models may be massive spin-1/2 objects. This again is a possibility which could be looked for experimentally or verified by numerical simulations.

The field theories for general  $\delta$  in both the spiral and colinear phases are still open questions. Although the results are qualitatively expected to be similar to the  $\delta = 0$  case in the spiral phase and the  $\delta = 1$  case in the colinear case, quantitative features such as the dependence of the gap on the coupling strengths will require the explicit form of the field theory.

## References

- [1] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983); Phys. Lett. A **93**, 464 (1983).
- [2] I. Affleck in *Fields, Strings and Critical Phenomena*, eds. E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1989); I. Affleck, J. Phys. Cond. Matt. **1**, 3047 (1989); Nucl. Phys. B **257**, 397 (1985).
- [3] T. Dombre and N. Read, Phys. Rev. B **39**, 6797 (1989).

- [4] P. Azaria, B. Delamotte, and D. Mouhanna, Phys. Rev. Lett. **68**, 1762 (1992); P. Azaria, B. Delamotte, T. Jolicouer, and D. Mouhanna, Phys. Rev. B **45**, 12612 (1992).
- [5] S. Rao and D. Sen, Nucl. Phys. B **424**, 547 (1994).
- [6] D. Allen and D. Senechal, Phys. Rev. B **51**, 6394 (1995).
- [7] D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988); D. Yoshioka, J. Phys. Soc. Jpn. **58**, 32 (1989); S. Sarkar, C. Jayaprakash, H. R. Krishnamurthy, and M. Ma, Phys. Rev. B **40**, 5028 (1989).
- [8] S. Rao and D. Sen, Phys. Rev. B **48**, 12763 (1993); R. Chitra, S. Rao, D. Sen, and S. S. Rao, Phys. Rev. B. **52**, 1061 (1995).
- [9] I. Affleck and J. B. Marston, Phys. Rev. B **37**, 3774 (1988); J. B. Marston and I. Affleck, Phys. Rev. B **39**, 11538 (1989); X. G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B, 11413 **39** (1989).
- [10] R. R. P. Singh and M. P. Gelfand, Phys. Rev. Lett. **61**, 2133 (1988).
- [11] T. Tonegawa and I. Harada, J. Phys. Soc. Jpn. **56**, 2153 (1987); I. Affleck, D. Gepner, H. J. Schulz, and T. Ziman, J. Phys. A **22**, 511 (1989); K. Okamoto and K. Nomura, Phys. Lett. A **169**, 433 (1992).
- [12] S. R. White and D. A. Huse, Phys. Rev. B **48**, 3844 (1993); S. R. White, Phys. Rev. B **48**, 10345 (1993); Y. Kato and A. Tanaka, J. Phys. Soc. Jpn. **63**, 1277 (1994).
- [13] R. Chitra, S. Pati, H. R. Krishnamurthy, D. Sen, and S. Ramasesha, Phys. Rev. B **52**, 6581 (1995); S. Pati, R. Chitra, D. Sen, H. R. Krishnamurthy, and S. Ramasesha, preprint no. cond-mat/9507129, to appear in Europhys. Lett. (1995).
- [14] S. H. Glarum, S. Geschwind, K. M. Lee, M. L. Kaplan, and J. Michel, Phys. Rev. Lett. **67**, 1614 (1991); S. Ma, C. Broholm, D. H. Reich, B. J. Sternlieb, and R. W. Erwin, Phys. Rev. Lett. **69**, 3571 (1992).
- [15] S. Rao and D. Sen, preprint no. cond-mat/9506145.

- [16] D. Senechal, Phys. Rev. B **52**, 15319 (1995); G. Sierra, preprint no. cond-mat/9512007.
- [17] We use the word ‘phase’ for convenience to denote the position of the peak in the spin-spin correlation function  $S(q)$ . There is actually no phase transition in the spin chain even at zero temperature.
- [18] J. Villain, J. Phys. (Paris) **35**, 27 (1974).
- [19] E. Ogievetsky, N. Reshetikhin, and P. Wiegmann, Nucl. Phys. B **280**, 45 (1987).
- [20] P. W. Anderson, Phys. Rev. **86**, 694 (1952); M. J. Klein and R. S. Smith, Phys. Rev. **80**, 1111 (1950).
- [21] E. Fradkin, *Field Theories of Condensed Matter Systems* (Addison-Wesley, Reading, 1991); E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).
- [22] For details of the derivation of the  $\beta$ -functions, see [5].
- [23] See S. R. White and D. A. Huse in [12].
- [24] E. H. Lieb, T. Schultz, and D. J. Mattis, Ann. Phys. (NY) **16**, 407 (1961); I. Affleck and E. H. Lieb, Lett. Math. Phys. **12**, 57 (1986).
- [25] F. D. M. Haldane, Phys. Rev. Lett. **61**, 1029 (1988); D. Loss, D. P. DiVincenzo and G. Grinstein, Phys. Rev. Lett. **69**, 3232 (1992) 3232; J. von Delft and C. L. Henley, *ibid.* **69**, 3236 (1992).
- [26] S. R. White, R. M. Noack, and D. J. Scalapino, Phys. Rev. Lett. **73**, 886 (1994); T. Barnes, E. Dagotto, J. Riera, and E. S. Swanson, Phys. Rev. B **47**, 3196 (1993); S. P. Strong and A. J. Millis, Phys. Rev. Lett. **69**, 2419 (1992).
- [27] M. K. T. Ami, M. Crawford, R. Harlow, Z. Wang, D. C. Johnston, Q. Huang, and R. Erwin, Phys. Rev. B **51**, 5994 (1995).

## Figure Captions

1. Classical phase diagram of the  $J_1 - J_2 - \delta$  spin chain.
2. Plot of  $\ln(\zeta/a)/S$  versus  $J_2/J_1$  for  $\delta = 0$ . For  $4J_2/J_1 < 1$ ,  $\ln(\zeta/a)$  is given by the one-loop RG of the  $O(3)$  NLSM for integer spin. For  $4J_2/J_1 > 1$ ,  $\ln(\zeta/a)$  is given by the one-loop RG of the  $SO(3)_L \times SO(2)_R$  NLSM.

Fig. 1

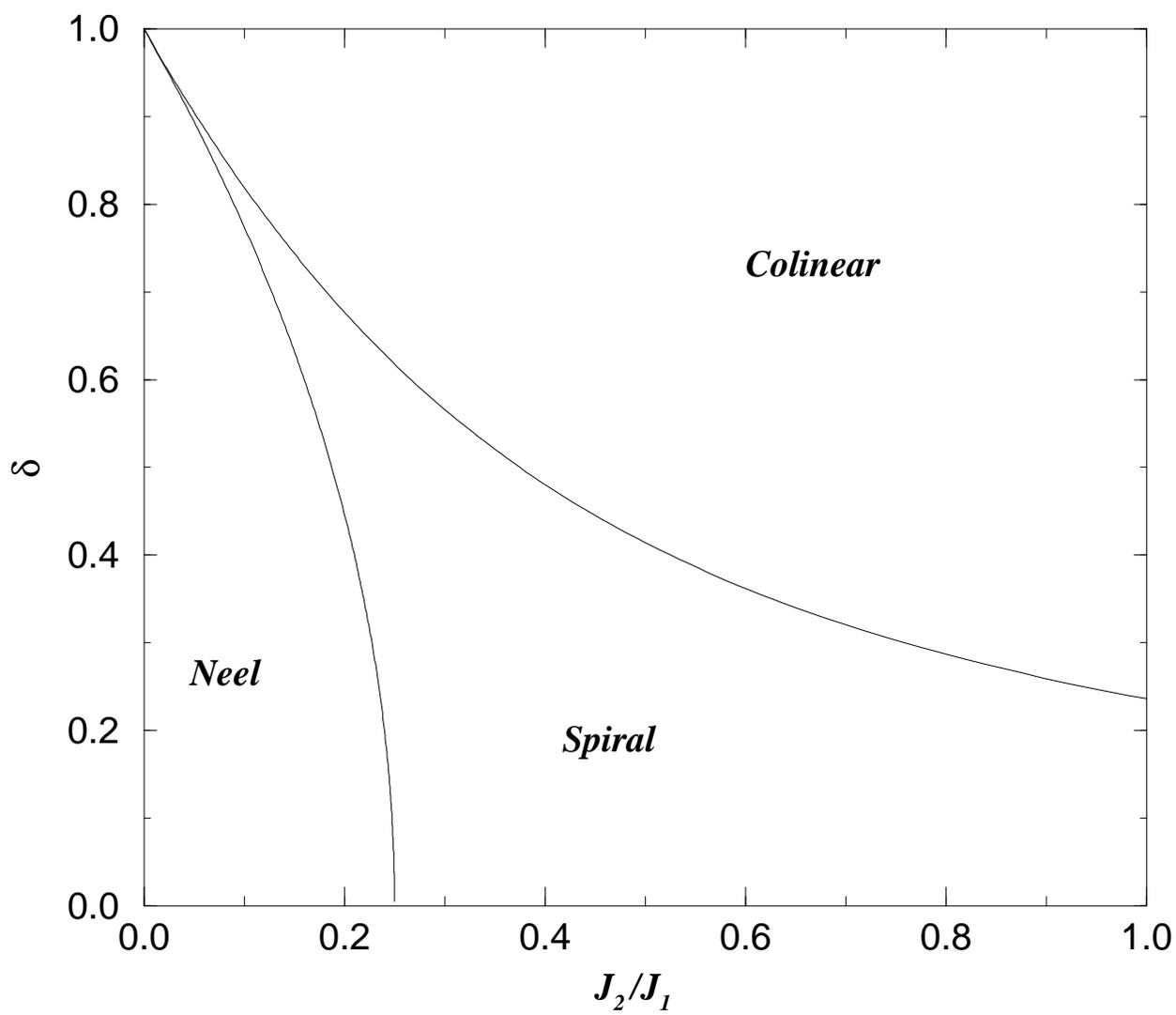


Fig. 2

