Field Theories of Frustrated Antiferromagnetic Spin Chains

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Abstract

We study the Heisenberg antiferromagnetic chain with both dimerization and frustration. The classical ground state has three phases: a Neel phase, a spiral phase and a colinear phase. In each phase, we discuss a non-linear sigma model field theory governing the low energy excitations. We study the theory in the spiral phase in detail using the renormalization group. The field theory, based on an $SO(3)$ matrix-valued field, becomes $SO(3) \times SO(3)$ and Lorentz invariant at long distances where the elementary excitation is analytically known to be a massive spin-1/2 doublet. The field theory supports Z_2 solitons which lead to a double degeneracy in the spectrum for half-integer spins (when there is no dimerization).

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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 non-linear sigma model (NLSM) field theories [1-6], Schwinger boson mean field theories [7], fermionic mean field theories [8], series expansions [9], exact diagonalization of small systems [10], and the density matrix renormalization group (DMRG) method [11, 12]. In one dimension, NLSM theories in particular have received special attention ever since Haldane [1] conjectured that integer spin models would have a gap, contrary to the known solution for the spin-1/2 model, and this prediction was verified experimentally [13].

In this Letter, we study a general Heisenberg spin chain with both dimerization (an alternation δ of the nearest neighbor (nn) couplings) and frustration (a next-nearest neighbor (nnn) coupling J_2). Even classically (*i.e.*, in the limit where the spin $S \to \infty$), the system has a rich ground state 'phase diagram', with three distinct phases, a Neel phase, a spiral phase and a colinear phase (defined below) [14]. For large but finite S, long wavelength fluctuations about the classical ground state can be described by non-linear field theories. These field theories are explicitly known in the Neel phase [1, 2] and in the spiral phase (for $\delta = 0$) [5, 6]. While the Neel phase has been extensively studied, various aspects like the ground state degeneracy and the low energy spectrum are not yet well understood in the spiral phase.

We will first discuss the field theory in the Neel phase for arbitrary J_2 and δ. For the spiral phase, we show using a one-loop renormalization group (RG) analysis that the field theory flows to an $SO(3) \times SO(3)$ symmetric and Lorentz invariant theory with an analytically known spectrum [15]. We also discuss how the presence of Z_2 solitons (supported by the field theory) affects the ground state degeneracy and the low energy spectrum. Finally, we show that the field theory in the colinear phase is qualitatively similar to the one in the Neel phase.

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

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

where $\mathbf{S}_i^2 = S(S+1)\hbar^2$, the coupling constants $J_1, J_2 \geq 0$ and the dimerization parameter 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

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

where θ_1 is the angle between the spins $\mathbf{S}_{2i}$ and $\mathbf{S}_{2i+1}$ and θ_2 is the angle between the spins $\mathbf{S}_{2i}$ and $\mathbf{S}_{2i-1}$. Minimization of the classical energy with respect to the θ_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 θ_1 and θ_2 are given by

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

where $\pi/2 < \theta_1 < \pi$ and $0 < \theta_2 < \pi$. 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 [16]. A detailed analysis will be presented elsewhere [17]. We only mention the qualitative results here. 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 distinction between the three phases is also brought out in the behavior of the spin-spin correlation function $S(q)$ in the classical limit. $S(q)$ is peaked 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 [12]. The colinear region has not yet been probed numerically.

The spin wave analysis is purely perturbative and is really not valid since there is no long-range order and no Goldstone modes in one dimension. To study non-perturbative aspects, we develop a NLSM to describe the low

energy modes. This is well-known in the Neel phase [1, 2]. The field variable is a unit vector $\vec{\phi}$ and the Lagrangian density is given by

$$\mathcal{L} \;=\; \frac{(\partial_t\vec{\phi})^2}{2cg^2} \;-\; \frac{c(\partial_x\vec{\phi})^2}{2g^2} \;+\; \frac{\theta}{4\pi}\;\vec{\phi}\cdot\partial_t\vec{\phi}\times\partial_x\vec{\phi}\;. \tag{4}$$

Here $c = 2J_1aS\sqrt{1-\delta^2-4J_2/J_1}$ is the spin wave velocity (a is the lattice spacing) and $g^2 = 2/(S\sqrt{1-\delta^2-4J_2/J_1})$ is the coupling constant. Note that large S corresponds to weak coupling. The third term in (4) is a topological term with $\theta = 2\pi S(1-\delta)$. This field theory is gapless for $\theta = \pi$ mod 2π 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 $\ln(\zeta/a) = \pi S\sqrt{1-\delta^2-4J_2/J_1}$. This is plotted in Fig. 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 $\theta_1 = \theta_2 = \theta = -J_1/(4J_2)$. 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 $i^{\rm th}$ site as $(\mathbf{S}_i)_a = S\sum_b \underline{R}_{ab}\mathbf{n}_b$, where $a, b = 1, 2, 3$ are the components along the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ axis, and $\mathbf{n}$ is a unit vector given by

$$\mathbf{n}_i \;=\; \frac{\hat{\mathbf{x}}\cos i\theta + \hat{\mathbf{y}}\sin i\theta + a\vec{\ell}}{\mid \hat{\mathbf{x}}\cos i\theta + \hat{\mathbf{y}}\sin i\theta + a\vec{\ell}\mid}\;. \tag{5}$$

The unit vector $\mathbf{n}_i$ describes the orientation of the $i^{\rm th}$ spin in the classical ground state (assumed to lie in the $\hat{\mathbf{x}}-\hat{\mathbf{y}}$ plane) and $\vec{\ell}$ represents the local magnetization. The Hamiltonian in Eq. (1) can be expanded in terms of $\underline{R}$ and $\vec{\ell}$ and Taylor expanded upto second order in space-time derivatives to obtain a continuum field theory [6]. The Lagrangian density is found to have an $SO(3)_L \times SO(2)_R$ symmetry and can be parametrized as

$$\mathcal{L} \;=\; \frac{1}{2c}\,{\rm tr}(\partial_t\underline{R}^T\partial_t\underline{R}\;P_0) \;-\; \frac{c}{2}\,{\rm tr}(\partial_x\underline{R}^T\partial_x\underline{R}\;P_1)\;, \tag{6}$$

where $c = J_1Sa(1+4J_2/J_1)\sqrt{1-J_1^2/16J_2^2}$, and P_0 and P_1 are diagonal matrices with entries given by

$$P_0 \;=\; \left(\frac{1}{2g_2^2},\;\frac{1}{2g_2^2},\;\frac{1}{g_1^2}-\frac{1}{2g_2^2}\right)$$

$$\text{and} \quad P_1 \quad = \quad \left(\frac{1}{2g_4^2}, \frac{1}{2g_4^2}, \frac{1}{g_3^2} - \frac{1}{2g_4^2} \right) . \tag{7}$$

The couplings g_i are found to be

$$\begin{aligned} g_2^2 &= g_4^2 = \frac{1}{S}\sqrt{\frac{4J_2 + J_1}{4J_2 - J_1}}, \\ g_3^2 &= 2g_2^2, \\ \text{and} \quad g_1^2 &= g_2^2 \left[1 + (1 - J_1/2J_2)^2 \right] . \end{aligned} \tag{8}$$

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 $g_1 g_4 \neq g_2 g_3$. 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 $\underline{R}(x) \to \underline{R}(-x)P$ 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. (8). 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 have computed the one-loop β-functions using the background field formalism [18]. (Note that since the theory is not Lorentz-invariant, geometric methods cannot be used to obtain the β-functions [4].) The β-functions are given by

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

$$
\begin{aligned}
\beta(g_3) &= \frac{g_3^3}{8\pi}\left[\ \frac{g_3^2 g_1 g_2}{g_4^2}\frac{2}{g_1 g_4 + g_2 g_3}\ +\ 2g_1 g_3\ (\frac{1}{g_3^2} - \frac{1}{g_4^2})\ \right], \\
\text{and}\quad \beta(g_4) &= \frac{g_4^3}{8\pi}\left[\ g_3^3 g_1 (\frac{2}{g_3^2} - \frac{1}{g_4^2})^2\ +\ 4g_1 g_3\ (\frac{1}{g_4^2} - \frac{1}{g_3^2})\ \right]. \qquad (9)
\end{aligned}
$$

We have numerically investigated the flow of these couplings using the initial values $g_i(a)$ given in Eq. (8). 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 one-loop, ζ 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 $4J_2/J_1 \to 1$ from either side (the Neel phase for integer spin or the spiral phase for any spin), $\ln(\zeta/a) \to 0$, *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 δ, 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 ζ. 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. [15]. 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 [11, 12] 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. [19] to study a one magnon state in the Neel 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

$$\underline{R}_1(x,t) = \begin{pmatrix} \cos\theta(x) & \sin\theta(x) & 0 \\ -\sin\theta(x) & \cos\theta(x) & 0 \\ 0 & 0 & 1 \end{pmatrix} \underline{R}_0(x,t) \ , \tag{10}$$

where $\theta(x)$ goes from 0 to 2π as x goes from $-\infty$ to $+\infty$. (For convenience, we choose $\theta(x) = 2\pi - \theta(-x)$, *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 2π 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 $U = \exp(\frac{i\pi}{2m+1}\sum_{n=-m}^{m}(2n+2m+1)S_n^z)$, then $\underline{R}_0(x,t)$ and $\underline{R}_1(x,t)$ have opposite parities because under parity, $S_i^z \to -S_i^z$ and $U \to U\exp(i2\pi\sum_{n=-m}^{m} S_n^z)$. 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 [20]. 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 [21]. 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 [22] 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 mod 2π if S is an integer and π mod 2π 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 [17]). 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 [12] (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.

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 [23]. The

field theory in this limit can be derived using the classical periodicity under translation by four lattice sites, similar to the derivation in Ref. [2] for the Neel phase. For two pairs of spins, we define

$$\vec{\phi}(x) = \frac{\mathbf{S}_{4i} - \mathbf{S}_{4i+1}}{2S}, \qquad \vec{\ell}(x) = \frac{\mathbf{S}_{4i} + \mathbf{S}_{4i+1}}{2a} ,$$
$$\text{and} \quad \vec{\phi}(x) = \frac{\mathbf{S}_{4i+3} - \mathbf{S}_{4i+2}}{2S} , \quad \vec{\ell}(x) = \frac{\mathbf{S}_{4i+3} + \mathbf{S}_{4i+2}}{2a} . \tag{11}$$

We 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 (4) *without* a topological term. We now have $c = 4aS\sqrt{J_2(J_2+J_1)}$ 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 [23].

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. It would be interesting to find an experimental system with sufficient frustration and dimerization to probe the colinear phase. This phase 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.

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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

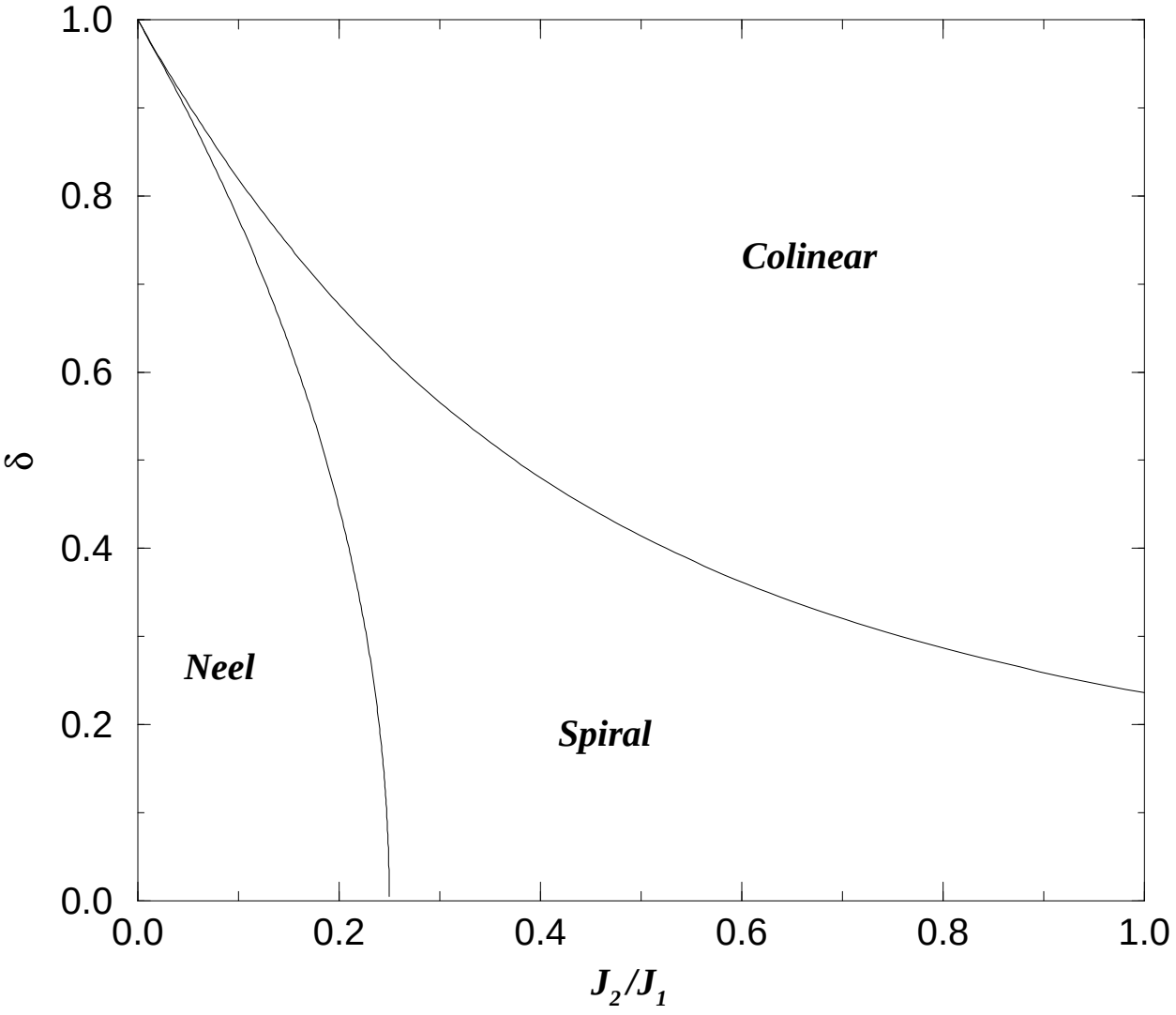

Fig. 2