# Phase Diagram of the Spin-One Heisenberg System with Dimerization and Frustration

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**Abstract**

We use the density matrix renormalization group method to study the ground state properties of an antiferromagnetic spin-1 chain with a next-nearest neighbor exchange $J_2$ and an alternation $\delta$ of the nearest neighbor exchanges. We find a line running from a gapless point at $(J_2, \delta) = (0, 0.25 \pm 0.01)$ upto an almost gapless point at $(0.725 \pm 0.01, 0$ such that the open chain ground state is 4-fold degenerate below the line and is unique above it. A disorder line $2J_2 + \delta = 1$ runs from $\delta = 0$ to about $\delta = 0.136$. To the left of this line, the peak in the structure factor $S(q)$ is at $\pi$, while to the right of the line, it is at less than $\pi$.

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While the isotropic spin-1/2 Heisenberg antiferromagnetic chain has been extensively studied using a variety of analytical and numerical techniques [1], the corresponding spin-1 chain has been studied in much less detail [2-4]. Interest in spin-1 chains grew after Haldane's conjecture that integer spin chains with a nearest-neighbor (nn) exchange should have a gap while half-integer spin chains should be gapless. This observation was based on a non-linear sigma model (NLSM) field theory description of the low-energy excitations [5]. The NLSM approach can be generalized to include other features such as dimerization (an alternation $\delta$ of the nn exchanges) and a next-nearest-neighbor (nnn) exchange $J_2$ [6], and it leads to interesting predictions. For instance, the spin-1 model should exhibit a gapless point at some critical value of $\delta$. If the nnn exchange is large enough, the spin chain goes over from a Neel like "phase" [7] to a spiral "phase" and a different kind of NLSM field theory becomes applicable [8,9]. This predicts a gap for *all* values of the spin.

In a recent paper [10], we studied the $J_2 - \delta$ model for a spin-1/2 chain using the density matrix renormalization group (DMRG) method [2,11]. In this Letter, we extend this study to the spin-1 chain with both dimerization and frustration and compare our results with the field theoretic expectations. The major surprise which we discover is an almost gapless point at ($J_2 = 0.725,\ \delta = 0$) which is contrary to the field theory expectation. We suggest that this point may be close to a critical point which is described by a $SU(3)$ symmetric conformal field theory (CFT) [12,13].

We have studied both open and periodic chains with an even number of sites governed by the Hamiltonian

$$H \ = \ \sum_i \ [\ 1 \ - \ (-1)^i \ \delta \ ] \ \mathbf{S}_i \cdot \mathbf{S}_{i+1} \ + \ J_2 \ \sum_i \ \mathbf{S}_i \cdot \mathbf{S}_{i+2} \ . \tag{1}$$

with the limits of $i$ being interpreted as appropriate. We restrict our attention to the region $J_2 \ \geq 0$ and $0 \leq \delta \leq 1$. We study various regions in the $(J_2, \delta)$ plane using DMRG.

The DMRG technique involves systematically building up the chain to a desired number of sites starting from a very short chain by adding two sites at a time. The initial chain of $2n$ sites (with $n$ a small enough integer) is diagonalized exactly. The reduced density matrix for the left $n$ sites is computed from the ground state of the $2n$ chain Hamiltonian by integrating over the states of the right $n$ sites. This density matrix is diagonalized and a matrix representation of the $n$-site Hamiltonian is obtained in a truncated basis with $m$ basis vectors which are the eigenvectors of the density matrix corresponding to its $m$ largest eigenvalues. The Hamiltonian matrix for the $2n+2$ chain is then obtained in the $(2s+1)^2 m^2$ dimensional direct product subspace constructed using the truncated basis of the left and the right halves of the $2n$ chain and the full space of the two additional spins which are inserted in the middle. After obtaining the ground state of the $2n+2$ chain in the truncated basis, the density matrix of half the chain, now with $n+1$ sites, is computed. The procedure is repeated till one reaches the desired chain length $N$. The accuracy of the DMRG technique depends crucially on the number of eigenvalues of the density matrix, $m$, which are retained. We worked with $m = 100$ to 120 over the entire $J_2 - \delta$ plane after checking that the DMRG results obtained using these values of $m$ agree well with exact numerical diagonalizations of chains upto 14 sites. The chain lengths we studied varied from 150 sites for $J_2 > 0$ to 200 sites for $J_2 = 0$. We tracked our results as a function of $N$ to check that convergence had been reached well before 150 sites.

The "phase diagram" which we obtained is shown in Fig. 1. There is a solid line marked $A$ which runs from $(0.25, 0)$ to about $(0.22 \pm 0.02, 0.20 \pm 0.02)$ shown by a cross. Within our numerical accuracy, the gap is zero on this line and the correlation length $\xi$ is as large as the system size $N$. The rest of the phase diagram is gapped. However the gapped portion can be divided into different regions characterized by other interesting features. On the dotted lines marked $B$, the gap is finite. Although $\xi$ goes through a maximum when we cross $B$ from either side, its value is much smaller than $N$. There is

a dashed line $C$ extending from $(0.65, 0.05)$ to about $(0.725, 0)$ on which the gap is very small and $\xi$ is very large but not as large as $N$. Below the curve $ABC$, the ground state for an *open* chain has a four-fold degeneracy (consisting of $S = 0$ and $S = 1$), whereas it is unique above the curve ($S = 0$). The dashed line marked $D$ satisfies $2J_2 + \delta = 1$, has an exactly dimerized ground state, and extends from $(0, 1)$ to about $(0.432, 0.136)$. Below the curve $ABC$, there is a line $E$ which goes down to about $(0.39, 0)$. Across $D$ and $E$, the position of the peak in the structure factor decreases from $\pi$ (Neel) to less than $\pi$ (spiral). (The positions of all the above points have an uncertainty of $\pm 0.01$ unless otherwise stated). We will comment on all these features of the phase diagram below.

For reasons explained below, the (almost) gapless point at $(0.725, 0)$ is quite unexpected. So we have studied that point in more detail. In Fig. 2, we present a plot of the gap versus $J_2$ along the line $\delta = 0$. It is highly non-monotonic with a very small value at about $J_2 = 0.725$. Fig. 3 is a plot of the static structure factor $S(q)$ versus $q$ at four values of $J_2$ near that point. (We studied open chains with 150 sites). For $J_2 = 0.725$ and 0.735, we see a pronounced peak at about $q_{max} = 112^o$ . The peak decreases in height and becomes broader as one moves away from those two values of $J_2$ . We estimate the maximum value of $\xi$ to be about 60 sites. It also decreases rapidly as we move away from those special values of $J_2$ .

It is natural to speculate that $(0.725, 0)$ lies close to some critical point which exists in a bigger parameter space. We believe that the appropriate critical point may be the one discussed in Refs. [12, 13]. Ref. 12 exactly solves a spin-1 chain which has nn interactions of the form

$$H \;=\; \sum_i \; [\; \vec{S}_i \cdot \vec{S}_{i+1} \;+\; (\; \vec{S}_i \cdot \vec{S}_{i+1} \;)^2 \;] \;, \tag{2}$$

and finds that there are gapless modes at $q = 0$ and $\pm\ 120^o$. This implies a peak in the structure factor at $q = 120^o$ which is not very far from the value we observe

numerically. Ref. 13 argues that the long-distance physics of this model is described by a CFT with $SU(3)$ symmetry [14].

Briefly, the field theoretic analysis of spin chains with the inclusion of $J_2$ and $\delta$ proceeds as follows. In the $S \to \infty$ limit, a classical treatment shows that the ground state of the model is in the Neel phase (a colinear configuration) for $4J_2 + \delta^2 < 1$, and in a coplanar spiral configuration for $4J_2 + \delta^2 > 1$. To next order in $1/S$, one derives a semiclassical field theory to describe the long-wavelength low-energy excitations. The field theory in the Neel phase is the $O(3)$ NLSM with a topological term [5,6]. The field variable is a unit vector $\vec{\phi}$ with the Lagrangian density

$$\mathcal{L} \;=\; \frac{1}{2cg^2}\;\dot{\vec{\phi}}^{\,2} \;-\; \frac{c}{2g^2}\;\vec{\phi}'^2 \;+\; \frac{\theta}{4\pi}\;\vec{\phi}\cdot\vec{\phi}'\times\dot{\vec{\phi}}\;, \tag{3}$$

where $c = 2S(1 - 4J_2 - \delta^2\ )^{1/2}$ is the spin wave velocity, $g^2 = 2/[S(1 - 4J_2 - \delta^2\ )^{1/2}]$ is the coupling constant, and $\theta = 2\pi S(1-\delta)$ is the coefficient of the topological term. Note that $\theta$ is independent of $J_2$ in the NLSM. (Time and space derivatives are denoted by a dot and a prime respectively). For $\theta = \pi \bmod 2\pi$ and $g^2$ less than a critical value, the system is gapless and is described by a CFT with an $SU(2)$ symmetry [6,13]. For any other value of $\theta$, the system is gapped. For $J_2 = \delta = 0$, one therefore expects that integer spin chains should have a gap while half-integer spin chains should be gapless. This is known to be true even for small values of $S$ like $1/2$ (analytically) and 1 (numerically) although the field theory is only derived for large $S$. In the presence of dimerization, one expects a gapless system at certain special values of $\delta$. For $S = 1$, the special value is predicted to be $\delta = 0.5$. We see that the *existence* of a gapless point is correctly predicted by the NLSM. However, according to the DMRG results, its location is at $\delta_c = 0.25$ for $J_2 = 0$ [3] and decreases with $J_2$ as shown in Fig. 1. These deviations from field theory are probably due to higher order corrections in $1/S$ which have not been studied analytically so far.

In the spiral phase, it is necessary to use a different NLSM which is known for

$\delta = 0$ [8,9]. The field variable is now an $SO(3)$ matrix $\underline{R}$ and the Lagrangian density is

$$\mathcal{L} \;=\; \frac{1}{2cg^2}\;\mathrm{tr}\;\Big(\;\dot{\underline{R}}^{T}\dot{\underline{R}}\;P_0\;\Big)\;-\;\frac{c}{2g^2}\;\mathrm{tr}\;\Big(\;\underline{R}'^{T}\underline{R}'\;P_1\;\Big), \tag{4}$$

where $c = S(1+y)\sqrt{1-y^2}/y$, $g^2 = 2\sqrt{(1+y)/(1-y)}/S$ with $1/y = 4J_2$ , and $P_0$ and $P_1$ are diagonal matrices with entries $(1, 1, 2y(1-y)/(2y^2-2y+1))$ and $(1, 1, 0)$ respectively. Note that there is no topological term; indeed, none is possible since $\Pi_2(SO(3)) = 0$ unlike $\Pi_2(S^2) = Z$ for the NLSM in the Neel phase. Hence there is no apparent difference between integer and half-integer spin. A one-loop renormalization group [8] and large $N$ analysis [9] then indicate that the system should have a gap for all values of $J_2$ and $S$, and that there is no reason for a particularly small gap at any special value of $J_2$ . (A similar conclusion is obtained from a bosonic mean-field theory analysis of the frustrated spin chain [15]). The almost gapless point at $J_2 = 0.725$ for spin-1 is therefore surprising.

For $\delta < 0.25$ and $J_2 = 0$, the spin-1 chain is known to exhibit a 'hidden' $Z_2 \times Z_2$ symmetry breaking described by a non-local order parameter [3,16]. This leads to a four-fold degeneracy of the ground state for the open chain. The degeneracy may be understood in terms of spin-1/2 degrees of freedom living at the ends of an open chain whose mutual interaction decreases exponentially with the chain length [17]. We have oberved this ground state degeneracy at all points below the curve $ABC$ in Fig. 1, where the gap between the singlet and triplet states vanishes exponentially with increasing chain length. Above the curve, the ground state is unique. The situation is reminiscent of the $Z_2 \times Z_2$ symmetry breaking mentioned above. However, we have not yet directly studied the non-local order parameter using DMRG.

We have also examined the structure factor $S(q)$. Since there is no long-range order anywhere in the $J_2 - \delta$ plane (except for algebraic order on the line $A$ in Fig. 1), $S(q)$ generally has a broad peak at some $q_{max}$ . To the left of lines $D$ and $E$ in Fig. 1, $q_{max}$ is pinned at $\pi$, while to the right of $D$ and $E$, $q_{max} < \pi$. Above the curve $ABC$,

the cross-over from the Neel to the spiral phase presumably occurs across the straight line $2J_2 + \delta = 1$ (see below). Below $ABC$, the cross-over has been determined purely numerically and seems to occur across the line indicated as $E$ in Fig. 1. The region of intersection between the cross-overs from Neel to spiral and from four-fold degeneracy to a unique ground state is a small 'hole' in the phase diagram centred about the point $(0.435, 0.12)$. Points in this 'hole' turned out to be extremely difficult to study using DMRG because of poor convergence with increasing chain lengths.

The segment $D$ of the straight line $2J_2 + \delta = 1$ indicated in Fig. 1 can be shown to have a dimerized state as the exact ground state. It is easy to show that a dimerized state of the form

$$\psi \;=\; [1,2]\;[3,4]\;....\;[N-1,N]\;, \tag{5}$$

where $[i,j]$ denotes the normalized singlet combination of the spins on sites $i$ and $j$, is an eigenstate of the Hamiltonian on that line. To prove that (5) is the ground state, we decompose the Hamiltonian as

$$H \;=\; \sum_i \; H_i\;, \tag{6}$$

where each of the $H_i$ only acts on a cluster of $n$ neighboring sites. Next, we numerically show that (5) is a ground state of each of the $H_i$ , and is therefore a ground state of $H$ by the Rayleigh-Ritz variational principle. For $n = 3$, this proof that (5) is the ground state works down to $\delta = 1/3$ [18]. Below that, (5) is no longer the ground state of any of the 3-cluster Hamiltonians $H_i$ . But we can construct 4-cluster $H_i$ satisfying (6) such that (5) can be numerically shown to be a ground state of each of those. This allows us to prove that (5) is the ground state of $H$ upto a point which is further down the line $D$. By repeating this calculation with bigger and bigger cluster sizes $n$, we can show that (5) is the ground state down to about $\delta = 0.136$. At that value of $\delta$, the cluster size $n$ is as large as the largest system sizes $N$ that we we have studied. Hence the argument that (5) is the ground state cannot be continued any further. Below

$\delta = 0.136$, we have the 'hole' where computations are difficult. Since the segment of the straight line from the point $(0, 1)$ upto the 'hole' has an exactly known ground state with an extremely short correlation length (essentially, one site), and since there is a cross-over from a Neel phase to a spiral phase across the line, we may call it a disorder line just as in the spin-1/2 case [10].

To summarize, we have studied a two-dimensional phase diagram for the ground state of an isotropic antiferromagnetic spin-1 chain. It is considerably more complicated than the corresponding spin-1/2 chain [10] with surprising features like an almost gapless point inside the spiral phase. We have suggested that this point is close to a critical point of a particular kind. It would be interesting to establish this more definitively. In any case, our results show that frustrated spin chains with small values of $S$ may exhibit features not anticipated from large $S$ field theories.

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**Figure Captions**

1. Phase diagram for spin-1 in the $(J_2, \delta)$ plane. The solid line $A$ extending from $(0.25, 0)$ upto the cross is gapless. The rest of the diagram is gapped. On the dotted lines $B$, the gap is finite. The dashed line $C$ close to $(0.725, 0)$ is almost gapless. The ground state for an open chain has a four-fold degeneracy below the curve $ABC$, while it is unique above $ABC$. The straight line $D$ satisfying $2J_2 + \delta = 1$ extends from $(0, 1)$ to about $(0.432, 0.136)$. Below $ABC$, there is a line $E$ which goes down to about $(0.39, 0)$. Across $D$ and $E$, the position of the peak in the structure factor decreases from $\pi$ (Neel) to less than $\pi$ (spiral).
2. Dependence of the gap on $J_2$ for $\delta = 0$.
3. Structure factor $S(q)$ versus $q$ for $J_2 = 0.71$, 0.72, 0.725 and 0.735 at $\delta = 0$.