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

Swapan Pati*, R. Chitra**, Diptiman Sen†,+, H. R. Krishnamurthy**,+ and S. Ramasesha*,+

* Solid State and Structural Chemistry Unit, 
Indian Institute of Science, Bangalore 560012, India

** Physics Department, Indian Institute of Science, 
Bangalore 560012, India

† Centre for Theoretical Studies, Indian Institute of Science, 
Bangalore 560012, India

‡ Jawaharlal Nehru Centre for Advanced Scientific Research, 
Indian Institute of Science Campus, Bangalore 560012, India

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

$$H = \sum_i \left[1 - (-1)^i \delta \right] \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}.$$  \hspace{1cm} (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 $2^n$ 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 $(2s+1)^2m^2$ 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 $q_{max} = 112^\circ$. 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

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

and finds that there are gapless modes at $q = 0$ and $\pm 120^\circ$. This implies a peak in the structure factor at $q = 120^\circ$ 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

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

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 $\theta = \pi \mod 2\pi$ 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
\[ \delta = 0 \text{ [8,9]. The field variable is now an } SO(3) \text{ matrix } R \text{ and the Lagrangian density is} \]

\[ L = \frac{1}{2cg^2} \text{ tr } \left( \dot{R}^T \dot{R} P_0 \right) - \frac{c}{2g^2} \text{ tr } \left( R'^T R' P_1 \right), \]  

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 observed 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

$$\psi = [1, 2][3, 4] .... [N - 1, N],$$

(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

$$H = \sum_i H_i,$$

(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 $H$ up to 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 \((0,1)\) up to 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 \((0.25, 0)\) up to 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 \(\delta = 0\).