A comparative study of the phase diagrams of spin-$\frac{1}{2}$ and spin-1 antiferromagnetic chains with dimerization and frustration

Swapan Pati[1], R. Chitra[2], Diptiman Sen[3,5],
S. Ramasesha[1,5] and H. R. Krishnamurthy[4,5]

[1] *Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012, India*
[2] *Laboratoire de Physique des Solides, Universite Paris-Sud, Batiment 510, 91405 Orsay, France*
[3] *Centre for Theoretical Studies, Indian Institute of Science, Bangalore 560012, India*
[4] *Physics Department, Indian Institute of Science, Bangalore 560012, India*
[5] *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 'phase' diagram and some low-energy properties of isotropic antiferromagnetic spin-$\frac{1}{2}$ and spin-1 chains with a next-nearest neighbor exchange J_2 and an alternation δ of the nearest neighbor exchanges. In the spin-$\frac{1}{2}$ chain, the system is gapless for $\delta = 0$ and $J_2 < J_{2c} = 0.241$, and is gapped everywhere else in the $J_2 - \delta$ plane. At J_{2c}, for small δ, the gap increases as δ^α, where $\alpha = 0.667 \pm 0.001$. $2J_2 + \delta = 1$ is a disorder line. To the left of this line, the structure factor $S(q)$ peaks at $q_{max} = \pi$ (Neel 'phase'), while to the right, q_{max} decreases from π to $\pi/2$ (spiral 'phase') as J_2 increases. There is also a '$\uparrow\uparrow\downarrow\downarrow$ phase' for large values of both J_2 and δ. In the spin-1 case, we find a line running from a gapless point at $(J_2, \delta) = (0, 0.25 \pm 0.01)$ upto a 'gapless' point at $(0.73 \pm 0.005, 0)$ such that the open chain ground state is four-fold degenerate below the line and is

unique above it. There is a disorder line in this case also and it has the same equation as in the spin-$\frac{1}{2}$ case, but the line ends at about $\delta = 0.136$. Similar to the spin-$\frac{1}{2}$ case, to the left of this line, the peak in the structure factor is at π (Neel 'phase'), while to the right of the line, it is at less than π (spiral 'phase'). For $\delta = 1$, the system corresponds to a spin ladder and the system is gapped for all values of the interchain coupling for both spin-$\frac{1}{2}$ and spin-1 ladders.

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I. INTRODUCTION

While the spin-$\frac{1}{2}$ 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, 3, 4, 5]. Interest in spin-1 chains grew after Haldane conjectured 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 [6]. The NLSM approach can be generalized to include other features such as dimerization (an alternation δ of the nn exchanges) and a next-nearest-neighbor (nnn) exchange J_2 [7], and it leads to interesting predictions. For the spin-$\frac{1}{2}$ model, it predicts that the system should be gapless for $J_2 < J_{2c}$, for $\delta = 0$ and should be gapped for all nonzero δ. On the other hand, the theory predicts that the spin-1 model should exhibit a gapless line in the $J_2 - \delta$ plane for nonzero δ. If the nnn exchange is large enough, the spin chains go over from a Neel 'phase' [8] to a spiral 'phase' and a different kind of NLSM field theory becomes applicable [9, 10] which predicts a gap for *all* values of the spin.

Real spin-$\frac{1}{2}$ Heisenberg systems with both dimerization and frustration are now known [11]. However, the spin-1 analogs are yet to be synthesized. In what follows, we demonstrate that the spin-1 system exhibits a richer 'phase' diagram than the spin-$\frac{1}{2}$ system. It is hoped that this will provide motivation for experimental realizations of such higher spin systems.

In this paper, we present a detailed comparative study of spin-1 and spin-$\frac{1}{2}$ chains with both dimerization and frustration in the $J_2 - \delta$ plane using the density matrix renormalization group (DMRG) method [12, 13, 14]. The major surprise which we discover is a 'gapless' (to numerical accuracy) point at ($J_2 = 0.73,\ \delta = 0$), in the spin-1 case, 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 [15, 16].

II. THE DMRG METHOD AND THE 'PHASE' DIAGRAM

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

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

with the limits of summation 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 the DMRG method. The interactions are schematically shown in Fig. 1.

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 target 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 target 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. This algorithm is suited for studying an infinite system by extrapolation. There is a different algorithm suited to studying a system with a specific finite size N [12]; this iteratively improves the density matrices so that these matrices correspond to the actual density matrices of the target state of the corresponding fragments in the desired finite size chain. This finite size algorithm could also be used for a detailed study of a specific finite chain system. We have however chosen to extrapolate to the thermodynamic limit by employing the algorithm described earlier for the infinite system.

The DMRG method allows us to study a few low-lying states in a sector with a given value of the total spin component, S_z. The ground state is always the first (lowest energy) state in the $S_z = 0$ sector. The accuracy of

the DMRG method depends crucially on the number of eigenstates of the density matrix, m, which are retained. We have 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 with upto 16 sites for spin-1 [4] and 22 sites for spin-$\frac{1}{2}$ [17]. 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 and found that convergence is reached well before 150 sites in all cases. We find that the numerical results are much better convergent for open chains than for periodic chains, a feature generic to the DMRG technique [12, 18]. Hence the data shown in Figs. 2 to 8, particularly for spin-1 chains, are mainly based on open chain results.

The 'phase' diagrams which we obtain for spin-$\frac{1}{2}$ and spin-1 chains are shown in Figs. 2 and 3, respectively. In the spin-$\frac{1}{2}$ case, the system is gapless from $J_2 = 0$ to $J_{2c} = 0.241$ for $\delta = 0$, and is gapped everywhere else in the $J_2 - \delta$ plane. There is a disorder line, $2J_2 + \delta = 1$, such that the peak in the structure factor $S(q)$ is at $q_{max} = \pi$ to the left of the line, and decreases from π to $\pi/2$ with increasing J_2 to the right of the line (Fig. 4). Further, the correlation length ξ goes through a minimum on this line. (We have borrowed the term 'disorder line' from the language of classical statistical mechanics [19]).

In the spin-1 case (Fig. 3), the phase diagram is more complex. There is a solid line marked A which runs from $(0, 0.25)$ to about $(0.22\pm0.02, 0.20\pm0.02)$ shown by a cross. Within our numerical accuracy, the gap is zero on this line and the correlation length ξ 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 ξ goes through a maximum when we cross B in going from region II to region I or from region III to region IV, its value is much smaller than N. There is a dashed line C extending from $(0.65, 0.05)$ to about $(0.73, 0)$ on which the gap appears to be zero (to numerical accuracy), and ξ is very large but not as large as N. In regions II and III, the ground state for an *open* chain has a four-fold degeneracy (consisting of $S = 0$ and $S = 1$), whereas it is nondegenerate in regions I and IV with $S = 0$. The dashed line marked D is defined by $2J_2 + \delta = 1$, has an exactly dimerized ground state, and extends from $(0, 1)$ to about $(0.432, 0.136)$. The line E separating regions II and III begins at about $(0.39, 0)$ and extends upto the region V. In regions I and II, the peak in

the structure factor is at π (Neel), while in regions III and IV, the structure factor peaks at less than π (spiral). We will comment on all these features of the 'phase' diagrams below.

A. The frustrated spin chain (the line $\delta = 0$)

For spin-$\frac{1}{2}$, the system is gapless and has a unique ground state for weak frustration, i.e., $0 < J_2 < J_{2c} = 0.241$. Beyond J_{2c}, the system is gapped and has two ground states [13]; these are spontaneously dimerized [20].

For spin-1, the system is gapped for all J_2 except for the 'gapless' point at $(0.73, 0)$. For reasons explained in Sec. III, this 'gapless' point is quite unexpected. So we examine that point in more detail. Fig. 5 shows a plot of the gap versus J_2 for $\delta = 0$. It is non-monotonic and is 'gapless' at about $J_2 = 0.73$. In regions II and III, i.e., for $J_2 \leq 0.735$, the open chain ground state is found to be four-fold degenerate. By comparing the energies of the low-lying states in sectors with $S_z = 0, 1$ and 2, we find that the four ground states have $S = 0$ and 1. We therefore define the gap as the energy difference between the first state in the $S_z = 0$ sector and the *second* state with $S_z = 1$, since the gap to the first state with $S_z = 1$ is zero. This is the correct definition of the gap since the finite ground state degeneracy arising from the end states (an artifact of the open boundary conditions) does not contribute to thermodynamic properties. In region IV, i.e., for $J_2 > 0.735$, the ground state is found to be unique with $S = 0$. So the gap is defined as the energy difference between the first states in the $S_z = 0$ and $S_z = 1$ sectors. In all cases, we extrapolate the gap Δ to infinite system size by fitting it to N using the form $\Delta = A + B/N^{\alpha}$, and finding the best possible values of A, B and α for each J_2 [21].

Fig. 6 is a plot of the static structure factor $S(q)$ versus q at four values of J_2 in the neighborhood of 0.73 obtained from open spin-1 chain studies with 150 sites. For J_2 between 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 this interval. We estimate the maximum value of ξ to be about 60 sites. It also decreases rapidly as we move away from that interval. Interestingly, Tonegawa *et al* [4] did find a pronounced peak in $S(q)$ at $J_2 = 0.7$, although they did not investigate it further.

It is natural to speculate that $(0.73, 0)$ lies close to some critical point which exists in a bigger parameter space of spin-1 chains. We believe that

the appropriate critical point may be the one discussed in Refs. [15, 16]. Sutherland exactly solves a spin-1 chain which has a nn biquadratic interaction of the form

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

with $\beta = 1$, and finds that there are gapless modes at $q = 0$ and $\pm\ 120^o$ [15]. This implies a peak in the structure factor at $q = 120^o$ which is not very far from the value we observe numerically. Affleck [16] further argues that the long-distance physics of this model is described by a conformal field theory with $SU(3)$ symmetry [22].

B. Ground state degeneracy

For spin-$\frac{1}{2}$, the ground state is always unique except on the line $\delta = 0$ and $J_2 > 0.241$; for $J_2 > 0.241$, the ground state is two-fold degenerate.

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, 23]. This leads to a four-fold degeneracy of the ground state for the open chain. The degeneracy may be understood in terms of spin-$\frac{1}{2}$ degrees of freedom living at the ends of the open chain whose mutual interaction decreases exponentially with chain length [24]. We have oberved this ground state degeneracy at all points in regions II and III in Fig. 2, where the gap between the singlet and triplet states vanishes exponentially with increasing chain length. In regions I and IV, 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 the DMRG method.

C. Structure factor $S(q)$

We have examined the equal-time two-spin correlation function $C(r) = \langle \vec{S}_o \cdot \vec{S}_r \rangle$, as well its Fourier transform $S(q)$. Since there is no long-range order anywhere in the $J_2 - \delta$ plane (except for algebraic order on the lines A in Figs. 2 and 3), $S(q)$ generally has a broad peak at some q_{max} .

For spin-$\frac{1}{2}$, q_{max} is pinned at π in region I (Neel), decreases from π (near the straight line B) to $\pi/2$ (near the numerically found curve C) in region II

(spiral), and is pinned at $\pi/2$ in region III ($\uparrow\uparrow\downarrow\downarrow$). These features are found by studying the behavior of $S(q)$ on all the points marked in Fig. 2. We assign a point to the $\uparrow\uparrow\downarrow\downarrow$ 'phase' if the sign of $C(r)$ alternates as $++--$ for 40 consecutive sites in a 100 site chain.

For spin-1, in regions I and II in Fig. 2, q_{max} is pinned at π, while in regions III and IV, $q_{max} < \pi$. Above the curve ABC, the cross-over from the Neel to the spiral 'phase' presumably occurs across the straight line D given by $2J_2 + \delta = 1$ (see below). Below ABC, the cross-over has been determined purely numerically and seems to occur across the line indicated as E in Fig. 2. 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' (region V) 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 the DMRG method because of convergence difficulties with increasing chain length. We have not shown the $\uparrow\uparrow\downarrow\downarrow$ 'phase' in the diagram for spin-1. However, we do find that the boundary of this phase for spin-1 is closer to the large-S boundary (given below as $4J_2 = (1-\delta^2)/\delta$) than for spin-$\frac{1}{2}$.

D. Disorder lines

For spin-$\frac{1}{2}$, the straight line B ($2J_2 + \delta = 1$) indicated in Fig. 2 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

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

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 (3) is the ground state, we decompose the Hamiltonian as

$$H \;=\; \sum_i \; H_i\;, \tag{4}$$

where each of the H_i only acts on a cluster of 3 neighboring sites. Next, we numerically show that (3) 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 spin-1, the above proof that ψ in Eq. (3) is the ground state holds only between $\delta = 1$ and $\delta = 1/3$ [25], where each of the H_i is a 3-cluster

Hamiltonian. For $\delta < 1/3$ along the disorder line, ψ in (3) is no longer the ground state of any of the 3-cluster Hamiltonians H_i . But we can construct 4-cluster H_i satisfying (4) such that ψ in (3) can be numerically shown to be a ground state of each of the H_i . This allows us to prove that ψ in (3) is the ground state of H upto a point which is further down the line D. By repeating this procedure with bigger and bigger cluster sizes n, we can show that ψ in (3) is the ground state down to about $\delta = 0.136$. At that value of δ, the cluster size n is as large as the largest system sizes that we have studied by the DMRG method. Hence the argument that (3) is the ground state could not be continued further. The difficulty is augmented by the fact that below $\delta = 0.136$, we have the 'hole' (region V) where computations are not convergent. 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 to a spiral 'phase' across the line, we choose to call it a disorder line just as in the spin-$\frac{1}{2}$ case [13].

Our DMRG studies show that the disorder line D does not extend below the 'hole' region; instead a new line E emerges as the disorder line. It is worthwhile noting that the line E is found only numerically unlike line D which is obtained analytically.

E. Coupled spin chains ($\delta = 1$)

For $\delta = 1$, we get two coupled spin chains as can be seen in Fig. 1; the interchain coupling is 2 and the intrachain coupling is J_2. We have scaled the intrachain coupling to 1, and have varied the interchain coupling J in these scaled units. We have studied the dependence of the gap Δ and the two-spin correlation function $C(r)$ on the interchain coupling J. We have plotted Δ versus J for both spin-$\frac{1}{2}$ and spin-1 in Fig. 7.

For spin-$\frac{1}{2}$, we find that the system is gapped for any non-zero value of the interchain coupling J, although the gap vanishes as $J \to 0$. We find that the gap increases and correspondingly the correlation length decreasess with increasing J.

For spin-1, we find the somewhat surprising result that both the gap and the correlation length ξ are fairly large for moderate values of J. Note that the variation of the gap with J for spin-1 (shown as circles) is much less than that for spin-$\frac{1}{2}$ (crosses). Fig. 8 shows the correlation function $C(r)$ as a

function of r for $J = 0.286$ for spin-1. This data is for an open ladder with 150 sites, and it is consistent with a value of ξ which is much longer than that found in the spin-$\frac{1}{2}$ case.

III. NLSM FIELD THEORIES OF ANTIFERROMAGNETIC SPIN CHAINS

A. The $J_2 - \delta$ model

Briefly, the field theoretic analysis of spin chains with the inclusion of J_2 and δ proceeds as follows. In the $S \to \infty$ limit, a classical treatment (explained briefly in the next subsection) shows that the ground state of the model is in the Neel phase for $4J_2 < 1 - \delta^2$, in a spiral phase for $1 - \delta^2 < 4J_2 < (1 - \delta^2)/\delta$, and in a '$\uparrow\uparrow\downarrow\downarrow$' phase for $(1 - \delta^2)/\delta < 4J_2$ [26] (Fig. 9). These three phases differ as follows. In the classical ground state, all the spins can be shown to lie in a plane. Let us define the angle between spins $\vec{S}_i$ and $\vec{S}_{i+1}$ to be θ_1 if i is odd and θ_2 if i is even. In the Neel phase, $\theta_1 = \theta_2 = \pi$. In the spiral phase, $\theta_1 = \theta_2 = \cos^{-1}(-1/4J_2)$ if $\delta = 0$. In the $\uparrow\uparrow\downarrow\downarrow$ phase, $\theta_1 = \pi$ and $\theta_2 = 0$.

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 given by a $O(3)$ NLSM with a topological term [6, 7]. The field variable is a unit vector $\vec{\phi}$ with the Lagrangian density

$$\mathcal{L} \;=\; \frac{1}{2cg^2}\;\dot{\vec{\phi}}^{\,2} \;-\; \frac{c}{2g^2}\;\vec{\phi}'^2 \;+\; \frac{\theta}{4\pi}\;\vec{\phi}\cdot\vec{\phi}'\times\dot{\vec{\phi}}\,, \tag{5}$$

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 θ 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 conformal field theory with an $SU(2)$ symmetry [7, 16]. For any other value of θ, 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 δ. For $S = 1$, the special value is predicted to be $\delta_c = 0.5$. We see that the *existence* of a gapless point is correctly predicted by the NLSM. However, according to the DMRG results, δ_c is at 0.25 for $J_2 = 0$ [3] and decreases with J_2 as shown in Fig. 3. 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 $\delta = 0$ [9, 10]. The field variable is now an $SO(3)$ matrix $\underline{R}$ and the Lagrangian density is

$$\mathcal{L} \;=\; \frac{1}{2cg^2}\;\mathrm{tr}\,\Big(\;\dot{\underline{R}}^{T}\,\dot{\underline{R}}\;P_0\;\Big)\;-\;\frac{c}{2g^2}\;\mathrm{tr}\,\Big(\;\underline{R}'^{T}\underline{R}'\;P_1\;\Big), \tag{6}$$

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 diagonal elements $(1, 1, 2y(1-y)/(2y^2-2y+1))$ 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 chains in the spiral phase. A one-loop renormalization group [9] and large N analysis [10] 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 [27]. The 'gapless' point at $J_2 = 0.73$ for spin-1 is therefore surprising.

In the $\uparrow\uparrow\downarrow\downarrow$ phase, the NLSM is known for $\delta = 1$, i.e., for the spin ladder. The Lagrangian is the same as in (5), with $c = 4S[J_2(J_2+1)]^{1/2}$ and $g^2 = (1+1/J_2)^{1/2}/S$. There is *no* topological term for any value of S, and the model is therefore gapped.

Note that the 'phase' boundary between Neel and spiral for spin-1 is closer to the the classical ($S \to \infty$) boundary $4J_2 = 1 - \delta^2$ than for spin-$\frac{1}{2}$. For instance, the crossover from Neel to spiral occurs, for $\delta = 0$, at $J_2 = 0.5$ for spin-$\frac{1}{2}$, at 0.39 for spin-1, and at 0.25 classically.

B. The frustrated and biquadratic spin-1 models

For spin-1, there is a striking similarity between the ground state properties of our model (1) as a function of J_2 (with $\delta = 0$) and the biquadratic

model (2) as a function of (positive) β [28]. For $J_2 < 0.39$ and $\beta < 1/3$, both models are in the Neel phase and are gapped. For $J_2 > 0.39$ and $\beta > 1/3$, the two models are in the spiral phase and are generally gapped; however, model (1) is 'gapless' for $J_2 = 0.73$ while model (2) is gapless for $\beta = 1$. We can qualitatively understand the cross-over from the Neel to the spiral phase (but *not* the gaplessness at a particular value of J_2 or β) through the following classical argument. Let us set the magnitudes of the spins equal to 1 and define the angle between spins $\vec{S}_i$ and $\vec{S}_{i+n}$ to be $n\theta$. The angle θ can be obtained by minimizing $\cos\theta + J_2 \cos 2\theta$ in (1), and $\cos\theta + \beta \cos^2\theta$ in (2). This gives us a Neel phase ($\theta = \pi$) if $J_2 \leq 1/4$ and $\beta \leq 1/2$ in the two models, and a spiral phase for larger values of J_2 and β with $\theta = \cos^{-1}(-1/4J_2)$ and $\theta = \cos^{-1}(-1/2\beta)$ respectively. The actual crossover points from Neel to spiral is different for spin-1 than these classical values.

IV. SUMMARY

To conclude, we have studied a two-parameter 'phase' diagram for the ground state of isotropic antiferromagnetic spin-$\frac{1}{2}$ and spin-1 chains. The spin-1 diagram is considerably more complex than the corresponding spin-$\frac{1}{2}$ chain with surprising features like a 'gapless' point inside the spiral 'phase'; this point could be close to a critical point discussed earlier in the literature [15, 16]. It would be interesting to establish this more definitively. Our results show that frustrated spin chains with small values of S exhibit features not anticipated from large S field theories.

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[21] For $J_2 \leq 0.735$, we also studied the separation between the second and the third states with $S_z = 1$. This separation is appreciably larger than the extent of non-monotonicity of the gap in the region around $J_2 = 0.5$. This confirms that the non-monotonic behaviour in that region is not an artifact arising from a possible mixing up of the first and second excited states in our diagonalization algorithm.

[22] At the $SU(3)$ symmetric critical point, the two-spin correlation should asymptotically decay as the 4/3 power of the distance [16]. We tried to verify this but the finite correlation length prevented us from obtaining an accurate estimate of the power.

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Figure Captions

1. Schematic picture of the spin chain given by Eq. (1).

2. 'Phase' diagram for the spin-$\frac{1}{2}$ chain in the $J_2 - \delta$ plane. The line A from $(0, 0)$ to $(0.241, 0)$ is gapless; the rest of the diagram is gapped. The straight line B satisfying $2J_2+\delta = 1$ extends all the way from $(0, 1)$ to $(0.5, 0)$. Across B, the position of the peak in the structure factor decreases from π (Neel) in region I to less than π (spiral) in region II. Across C, the peak in the structure factor decreases from greater than $\pi/2$ (spiral) in region II to $\pi/2$ in region III ($\uparrow\uparrow\downarrow\downarrow$ 'phase'). The two-spin correlation function and structure factor were studied at all the points shown in the figure.

3. 'Phase' diagram for the spin-1 chain. The solid line A extending from $(0, 0.25)$ 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 $(0.73, 0)$ is 'gapless'. The ground state for an open chain has a four-fold degeneracy in regions II and III, while it is unique in regions I and IV. The straight line D satisfying $2J_2 + \delta = 1$ extends from $(0, 1)$ to about $(0.432, 0.136)$. Regions II and III are separated by line E which goes down to about $(0.39, 0)$. Across D and E, the peak in the structure factor decreases from π (Neel) in regions I and II to less than π (spiral) in regions III and IV. The positions of all the points have an uncertainty of ± 0.01 unless stated otherwise.

4. Plot of q_{max} (in degrees) versus J_2 at $\delta = 0$ for spin-$\frac{1}{2}$.

5. Dependence of the gap on J_2 at $\delta = 0$ for spin-1.

6. Structure factor $S(q)$ versus q for $J_2 = 0.71$, 0.72, 0.725 and 0.735 at $\delta = 0$ for spin-1.

7. Gap Δ versus J for coupled spin chains ($\delta = 1$). Spin-$\frac{1}{2}$ and spin-1 data are indicated by crosses and circles respectively.

8. Two-spin correlation function $C(r)$ versus r for coupled spin-1 chains with $J = 0.286$.

9. Classical phase diagram of the spin chain in the $J_2 - \delta$ plane.