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

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Abstract. The ground-state 'phase' diagrams and some low-energy properties of isotropic antiferromagnetic spin-$\frac{1}{2}$ and spin-1 chains with a next-nearest-neighbour exchange J_2 and an alternation δ of the nearest-neighbour exchanges have been compared for the first time using the density matrix renormalization group method. 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–δ 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 $q_{max} = \pi$ (the Néel 'phase'), while to the right, q_{max} decreases from π to $\pi/2$ (the spiral 'phase') as J_2 increases. We also discover a '↑↑↓↓ 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 $(J_2, \delta) = (0, 0.25 \pm 0.01)$ up to a 'gapless' point at $(0.73 \pm 0.005, 0)$ such that the open-chain ground state is fourfold 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 $\delta = 0.136$. Similarly to the spin-$\frac{1}{2}$ case, to the left of this line, the peak in the structure factor is at π (the Néel 'phase'), while to the right of the line, it is at less than π (the 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.

1. Introduction

Antiferromagnetic spin-1 chains received fresh attention [1–4] after Haldane conjectured that integer-spin chains with a nearest-neighbour (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 δ of the nn exchanges) and a next-nearest-neighbour (nnn) exchange J_2 [6], 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 non-zero δ. On the other hand, the theory predicts that the spin-1 model should exhibit a gapless line in the J_2–δ plane for non-zero δ. If the nnn exchange is large enough, the spin chains go over from a Néel 'phase' [7] to a spiral 'phase' and a different kind of NLSM field theory becomes applicable [8, 9] which predicts a gap for *all* values of the spin.

While the spin-$\frac{1}{2}$ chain has been extensively studied using a variety of analytical and numerical techniques [10], the corresponding spin-1 chain has been studied in much less detail. Real spin-$\frac{1}{2}$ Heisenberg systems with both dimerization and frustration are now known [11]. However, the spin-1 analogues 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.

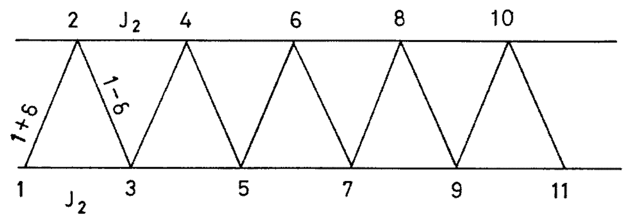

Figure 1. A schematic picture of the spin chain given by equation (1).

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–δ plane using the density matrix renormalization group (DMRG) method [12–14]. A major surprise which we discuss 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]. We also discuss a phase called '$\uparrow\uparrow\downarrow\downarrow$' which arises if both J_2 and δ are large. A particular case of this is the spin ladder ($\delta = 1$), and we present some numerical results for both spin-$\frac{1}{2}$ and spin-1 ladders.

2. 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

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

with the limits of summation being interpreted as appropriate. We restrict our attention to the region $J_2 \geqslant 0$ and $0 \leqslant \delta \leqslant 1$. We study various regions in the J_2–δ plane using the DMRG method which has proved to be very successful for one-dimensional quantum systems [12–14, 17]. The interactions are shown schematically in figure 1.

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–δ plane after checking that the DMRG results obtained using these values of m agree well with exact numerical diagonalizations of chains with up to 16 sites for spin-1 [3] and 22 sites for spin-$\frac{1}{2}$ [18]. The chain lengths that we studied varied from 150 sites for $J_2 > 0$ to 200 sites for $J_2 = 0$. We tracked our results as a

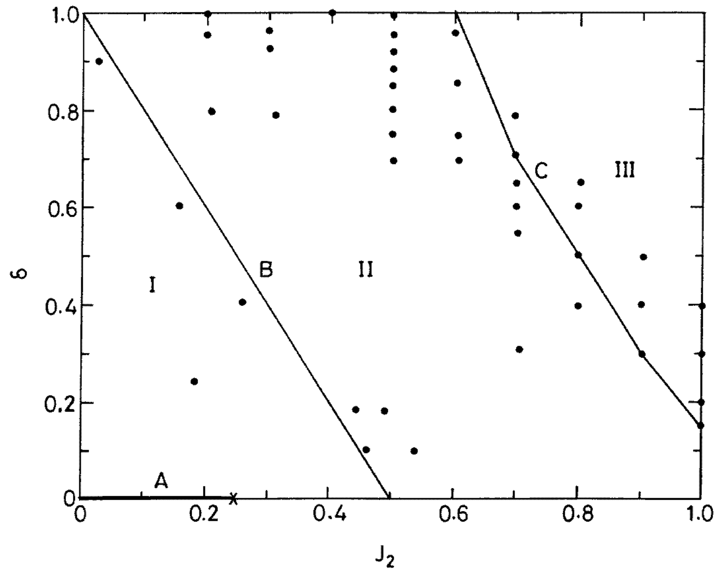

Figure 2. The 'phase' diagram for the spin-$\frac{1}{2}$ chain in the J_2–δ plane. The line A from $(0, 0)$ to $(0.241, 0)$ is gapless; the rest of the diagram is gapped. The straight line B satisfying $2J_2 + \delta = 1$ extends all the way from $(0, 1)$ to $(0.5, 0)$. Across B, the position of the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

function of N and found that convergence is reached well before 150 sites in all cases. We find that the numerical results converge much better for open chains than for periodic chains, a feature generic to the DMRG technique [12, 19]. Hence the data shown in figures 2 to 8 (see later), 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 figures 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–δ 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 (figure 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 [20].)

In the spin-1 case (figure 3), the phase diagram is more complex. There is a solid line marked A which runs from $(0, 0.25)$ 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 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 fourfold degeneracy (consisting of $S = 0$ and $S = 1$), whereas it is non-degenerate in

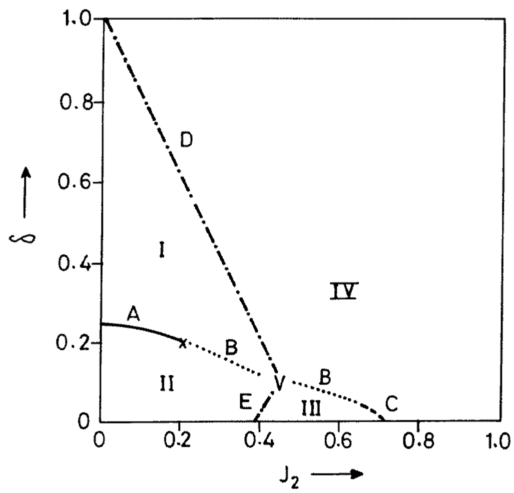

Figure 3. The 'phase' diagram for the spin-1 chain. The solid line A extending from $(0, 0.25)$ up to the cross is gapless; the rest of the diagram is gapped. On the dotted lines B, the gap is finite. The dashed line C close to $(0.73, 0)$ is 'gapless'. The ground state for an open chain has a fourfold 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 (the Néel phase) in regions I and II to less than π (the spiral phase) in regions III and IV. The positions of all the points have an uncertainty of ± 0.01 unless stated otherwise.

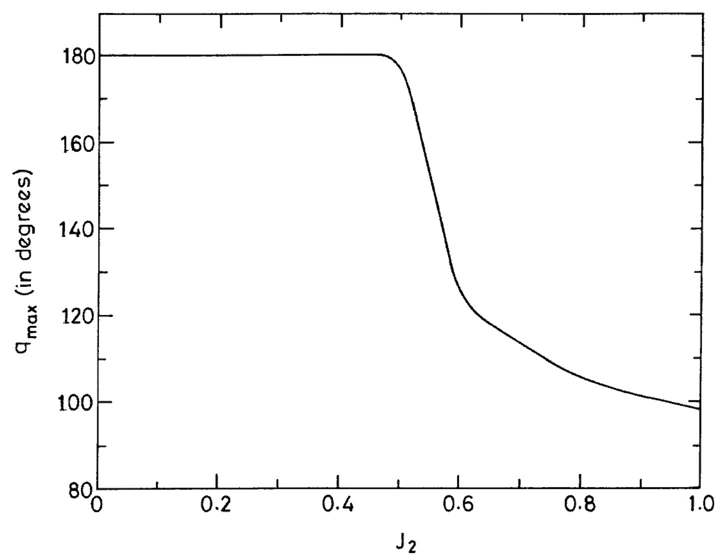

Figure 4. A plot of q_{max} (in degrees) versus J_2 at $\delta = 0$ for spin-$\frac{1}{2}$.

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 up to the region V. In regions I and II, the peak in the structure factor is at π (the Néel phase), while in regions III and IV, the structure factor peaks at less than π (the spiral phase). We will comment on all of these features of the 'phase' diagrams below.

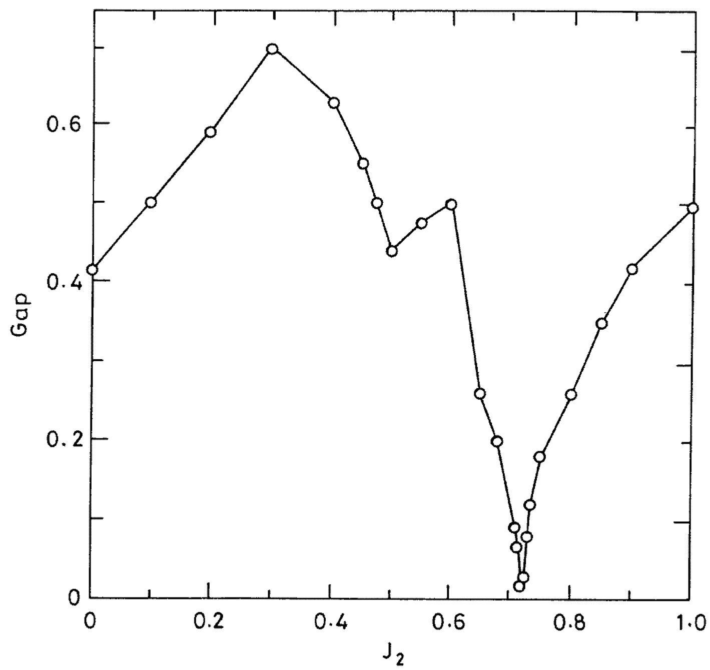

Figure 5. The dependence of the gap on J_2 at $\delta = 0$ for spin-1.

2.1. 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 [21].

For spin-1, the system is gapped for all J_2 except for the 'gapless' point at $(0.73, 0)$. For reasons explained in section 3, this 'gapless' point is quite unexpected. So we examine that point in more detail. Figure 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 $J_2 \leqslant 0.735$, the open-chain ground state is found to be fourfold 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 [22].

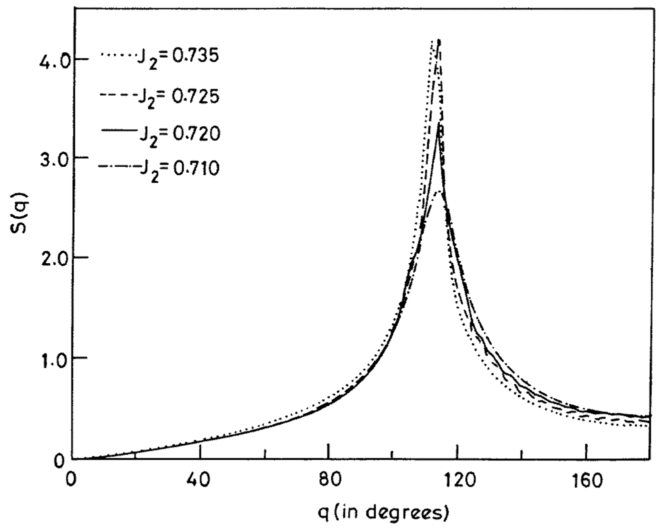

Figure 6. The structure factor $S(q)$ versus q for $J_2 = 0.71$, 0.72, 0.725 and 0.735 at $\delta = 0$ for spin-1.

Figure 6 is a plot of the static structure factor $S(q)$ versus q at four values of J_2 in the neighbourhood 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 $q_{max} = 112^\circ$. 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* [3] 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 references [15, 16]. Sutherland exactly solves a spin-1 chain which has a nn biquadratic interaction of the form

$$H = \sum_i [\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \beta(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2] \qquad (2)$$

with $\beta = 1$, and finds that there are gapless modes at $q = 0$ and $\pm 120^\circ$ [15]. This implies a peak in the structure factor at $q = 120^\circ$ which is not very far from the value that 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 [23].

2.2. 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 twofold 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 [2, 24]. This leads to a fourfold 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 [25]. We have observed this ground-state degeneracy at all points in regions II and III in figure 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.

2.3. The structure factor $S(q)$

We have examined the equal-time two-spin correlation function $C(r) = \langle \boldsymbol{S}_0 \cdot \boldsymbol{S}_r \rangle$, as well as its Fourier transform $S(q)$. Since there is no long-range order anywhere in the J_2–δ plane (except for algebraic order on the lines A in figures 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 (the Néel phase), decreases from π (near the straight line B) to $\pi/2$ (near the curve C found numerically) in region II (the spiral phase), and is pinned at $\pi/2$ in region III ($\uparrow\uparrow\downarrow\downarrow$). These features are found by studying the behaviour of $S(q)$ on all of the points marked in figure 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 figure 2, q_{max} is pinned at π, while in regions III and IV, $q_{max} < \pi$. Above the curve ABC, the crossover from the Néel to the spiral 'phase' presumably occurs across the straight line D given by $2J_2 + \delta = 1$ (see below). Below ABC, the crossover has been determined purely numerically and seems to occur across the line indicated as E in figure 2. The region of intersection between the crossovers from the Néel to the spiral phase and from fourfold 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-$\frac{1}{2}$.

Although one can easily show that the system must be in the $\uparrow\uparrow\downarrow\downarrow$ phase if $\delta = 1$, our numerical results show for the first time that the $\uparrow\uparrow\downarrow\downarrow$ phase also extends to the region $\delta < 1$. This agrees with the semiclassical arguments presented in section 3.

2.4. Disorder lines

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

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

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 three neighbouring 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 equation (3) is the ground state holds only between $\delta = 1$ and $\delta = 1/3$ [26], where each of the H_i is a three-cluster Hamiltonian. For $\delta < 1/3$ along the disorder line, ψ in (3) is no longer the ground state of any of the three-cluster

Hamiltonians H_i. But we can construct a four-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 up to 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 $(0, 1)$ up to the 'hole' has an exactly known ground state with an extremely short correlation length (essentially, one site), and since there is a crossover from a Néel 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.

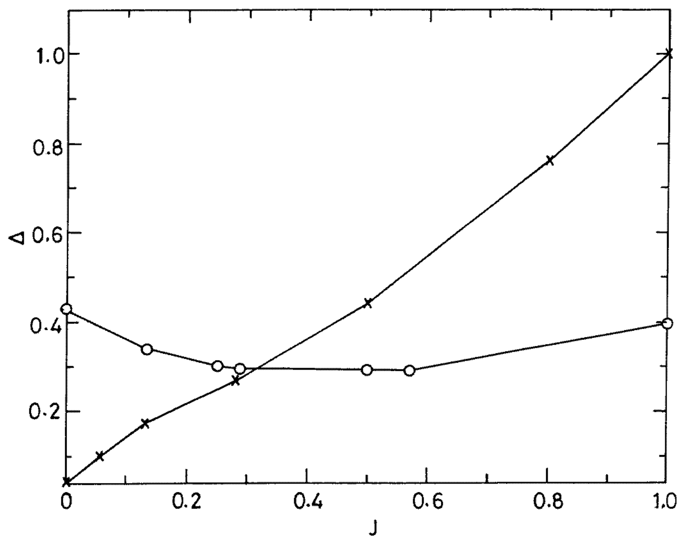

Figure 7. The gap Δ versus J for coupled spin chains ($\delta = 1$). Spin-$\frac{1}{2}$ and spin-1 data are indicated by crosses and circles respectively.

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

For $\delta = 1$, we get two coupled spin chains (also called a spin ladder) as can be seen in figure 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 figure 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 decreases with increasing J.

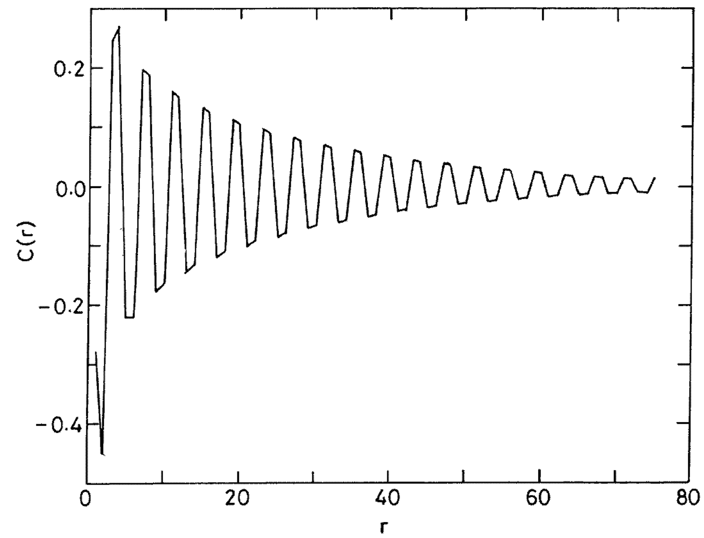

Figure 8. THe two-spin correlation function $C(r)$ versus r for coupled spin-1 chains with $J = 0.286$.

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). Figure 8 shows the correlation function $C(r)$ as a function of r for $J = 0.286$ for spin-1. This data are for an open ladder with 150 sites, and are consistent with a value of ξ which is much larger than that found in the spin-$\frac{1}{2}$ case. It would be useful to understand the reason for the large values of ξ for the spin-1 ladder, perhaps in terms of some variational wave functions analogous to the resonating-valence-bond wave functions for the spin-$\frac{1}{2}$ ladder [27].

3. NLSM field theories of antiferromagnetic spin chains

3.1. The J_2–δ 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 Néel 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 $(1 - \delta^2)/\delta < 4J_2$ [28] (figure 9). These three phases differ as follows. In the classical ground state, all of the spins can be shown to lie in a plane. Let us define the angle between spins $\boldsymbol{S}_i$ and $\boldsymbol{S}_{i+1}$ to be θ_1 if i is odd and θ_2 if i is even. In the Néel 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 the next order in $1/S$, one derives a semiclassical field theory to describe the long-wavelength low-energy excitations. The field theory in the Néel phase is given by an O(3) NLSM with a topological term [5, 6]. The field variable is a unit vector ϕ with the Lagrangian density

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

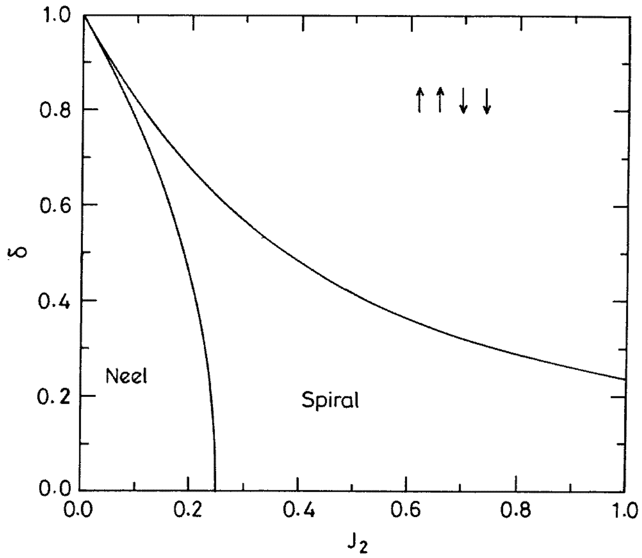

Figure 9. The classical phase diagram of the spin chain in the J_2–δ plane.

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 [6, 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 $J_2 = 0$ [2] and decreases with J_2 as shown in figure 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 $\delta = 0$ [8, 9]. The field variable is now an SO(3) matrix $\mathbf{R}$ and the Lagrangian density is

$$\mathcal{L} = \frac{1}{2cg^2}\mathrm{tr}(\dot{\mathbf{R}}^{\mathrm{T}}\dot{\mathbf{R}}P_0) - \frac{c}{2g^2}\mathrm{tr}(\mathbf{R}'^{\mathrm{T}}\mathbf{R}'P_1) \qquad (6)$$

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 $\Pi_2(\mathrm{SO}(3)) = 0$ in contrast to $\Pi_2(S^2) = \mathrm{Z}$ for the NLSM in the Néel phase. Hence there is no apparent difference between integer- and half-integer-spin chains in the spiral phase. A one-loop renormalization group [8] and large-N analysis [9] 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 [29]. The 'gapless' point at $J_2 = 0.73$ for spin-1 is therefore surprising.

In the ↑↑↓↓ 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 the Néel and the spiral phase for spin-1 is closer to the classical ($S \to \infty$) boundary $4J_2 = 1 - \delta^2$ than for spin-$\frac{1}{2}$. For instance, the crossover from the Néel to the spiral phase 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.

3.2. 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 [30]. For $J_2 < 0.39$ and $\beta < 1/3$, both models are in the Néel 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 crossover from the Néel 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 $\boldsymbol{S}_i$ and $\boldsymbol{S}_{i+n}$ 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 Néel phase ($\theta = \pi$) if $J_2 \leqslant 1/4$ and $\beta \leqslant 1/2$ 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 the Néel to the spiral phase are different for spin-1 to these classical values.

4. 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.

After this paper was accepted for publication, we learnt of a more detailed DMRG study of the frustrated spin-1 chain [31], which leads to somewhat different results for the various regions on the line $\delta = 0$.

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