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## Generalized Heisenberg Quantum Spin Chains (Invited)

Jill C. Bonner  
*University of Rhode Island*

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## Generalized Heisenberg quantum spin chains (invited)

Jill C. Bonner

*Department of Physics, University of Rhode Island, Kingston, Rhode Island 02881*

Since the Heisenberg spin chain can be considered the simplest realistic model of magnetism, surprise and some degree of controversy have resulted from recent work of Haldane. The prediction is that quantum spin chains with *half-integer* spin should all display  $T = 0$  phase behavior equivalent to that of the Bethe Ansatz integrable (solvable) spin-1/2 quantum chain. More remarkably, the class of *integer* spin chains is predicted to show very different phase behavior. In particular, a gap should be present in the spectrum of a Heisenberg antiferromagnetic chain. This remarkable feature is counterintuitive in terms of accepted wisdom in magnetism (spin-wave theory, spin-Peierls theory) and critical phenomena. Consequently the verification of the prediction is of great interest. A considerable amount of numerical work has been done, involving finite-chain, finite-size scaling, variational, Monte Carlo and other calculations, which will be reviewed here. The present consensus is that the weight of numerical evidence supports the prediction, although puzzling features still remain. Adding additional interactions to the basic Heisenberg Hamiltonian such as spin ( $XXZ$ ) anisotropy, single-ion anisotropy, biquadratic exchange, and an applied magnetic field, generates a rich and complicated phase diagram for chains with spin  $> 1/2$ , particularly for the case of integer spin. The  $s = 1$  phase diagram seems to display critical behavior of a type not previously encountered. A theoretical appraisal of the Haldane phenomenon will include a discussion of the possible role of nonintegrability. Mention will also be made of current progress in experimental investigation of the phenomenon, including problems that might be encountered. More recent work of Affleck has greatly generalized the field-theoretic mappings which underlay the original work of Haldane. A number of interesting problems have been mapped into quantum spin chains of various types, including field theoretic phenomena and the localization problem of the quantum Hall effect.

### INTRODUCTION

Considerable interest has been aroused in quantum spin chains of various spin values  $s$  because of a recent remarkable prediction by Haldane.<sup>1</sup> According to Haldane, the class of *integer-spin* Heisenberg-like antiferromagnetic (AFM) spin chains differs radically in its  $T = 0$  critical behavior from the class of *half-integer-spin* quantum spin chains. Subsequently, Affleck<sup>2-4</sup> on the basis of ideas related to those of Haldane, has produced a series of interesting mappings from two-dimensional (2D) classical continuum field theories to various types of quantum spin chain, including systems with integer spin, half-integer spin, spin anisotropy, and alternation. Affleck was able to relate the critical properties of these various chains to field-theoretic entities such as merons<sup>3</sup> and dyons<sup>4</sup> on the one hand, and to the localization length problem of the 2D quantum Hall effect on the other.<sup>2</sup> The purpose of this paper is to discuss the potential impact on the fields of magnetism and critical phenomena of these surprising predictions, and review the present status of numerical verification.

Until recently, it was generally believed that Heisenberg AFM quantum spin chains showed a generic resemblance to one another, independent of spin  $s$ , in general accordance with spin-wave theory.<sup>5</sup> According to Haldane, this is only

the case for chains with half-integer spin, which resemble the familiar spin-1/2 Heisenberg AFM chain.<sup>6</sup> Integer-spin Heisenberg chains, remarkably, are expected to show an excitation gap whose magnitude is related to the value of the spin. This has physical significance for spin-Peierls theory<sup>7</sup> and the behavior of alternating spin chains. Consider the uniform Heisenberg AFM Hamiltonian

$$H = J \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \quad (1)$$

and add a staggering term

$$\delta J \sum_{i=1}^N (-1)^i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

to give the alternating (dimerized) Hamiltonian

$$H = J \sum_{i=1}^N [(1 - \delta) \mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} + (1 + \delta) \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1}], \quad (2)$$

where  $\delta$  is known as the dimerization parameter. Taking the limit  $\delta = 0$  recovers the uniform Heisenberg chain, and  $\delta = 1$  corresponds to an assembly of noninteracting pairs of spins  $s$  (dimers). For the case of spin-1/2, a singlet-triplet excitation gap opens up in the spectrum for  $\delta > 0$  accompanied by lowering of the energy. This basic instability gives

rise to the spin-Peierls transition, where an assembly of uniform Heisenberg AFM chains with weak spin-lattice coupling undergoes a progressive, i.e., temperature-dependent, dimerization below the spin-Peierls transition temperature. According to Haldane, a spin-1 uniform Heisenberg AFM chain already has "alternating" character, i.e., a singlet-triplet excitation gap is present in the spectrum. Hence effective spin-1 systems are not expected to undergo spin-Peierls transitions.

Consider the spin- $s$  XXZ AFM Hamiltonian

$$H = J \sum_{i=1}^N (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z). \quad (3)$$

Here,  $\Delta$  is the spin anisotropy parameter, such that  $\Delta = 1$  recovers the isotropic Heisenberg limit,  $\Delta > 1$  corresponds to uniaxial (Ising-like) anisotropy, and  $0 \leq \Delta < 1$  to easy-plane anisotropy. Haldane specifically predicts that all half-integer- $s$  systems behave qualitatively like the Bethe Ansatz solvable spin-1/2 case, which is known to exhibit a gapless critical phase for  $0 \leq \Delta < 1$  and an AFM-ordered phase for  $\Delta > 1$ . The lowest-lying excitations for half-integer spin are shown schematically in Fig. 1(a), where the Heisenberg point  $\Delta = 1$  corresponds to an essential singularity, and an excitation gap opens up exponentially above the doubly degenerate ground state for  $\Delta > 1$ . For integer- $s$  systems, on the other hand, Haldane predicts the existence of a disordered singlet phase between the critical and the AFM-ordered phases. The singlet phase (characterized by a nonzero excitation gap) is realized for the anisotropy range  $\Delta_1 < \Delta < \Delta_2$ , where  $0 \leq \Delta_1 < 1$  and  $1 < \Delta_2$ , thus encompassing the Heisenberg point  $\Delta = 1$ . The lowest-lying excitations for integer spin are shown schematically in Fig. 1(b). The critical point  $\Delta_1$  corresponds to an essential singularity terminating a gapless phase, and the second critical point  $\Delta_2$  is predicted to correspond to the  $T = 0$  transition point at the critical field

of the spin-1/2 transverse Ising model. Strictly speaking, the mapping on which these predictions are based holds only the large  $s$  limit,<sup>8</sup> but numerical results suggest (a) a gap is present in the case of the lowest integer spin value  $s = 1$  and (b) a gap is barely detectable in the case of  $s = 2$ , in qualitative accordance with the Haldane formula<sup>1</sup>

$$\Delta E \sim JS^2 e^{-\pi s}. \quad (4)$$

In the case of more general spin chains, and as in the case of the Haldane prediction, on the basis of mappings from 2D classical continuum  $\sigma$  models (and related Wess-Zumino models), Affleck has made the following predictions.

### A. Alternating AFM chains<sup>2</sup>

The critical exponent of the localization length problem of the quantum Hall effect maps into the gap exponent of alternating spin chains in the  $s \rightarrow \infty$  limit. Specifically, the localization length  $\xi$  of the quantum Hall problem is given by<sup>2</sup>

$$\xi \sim |E - E_c|^{-\nu}, \quad (5)$$

and if the gap exponent of the alternating chain is defined as  $\Delta E \sim \delta^\phi$ , then

$$\phi = 4(1 + s)/(5 + 8s) \quad (6a)$$

and

$$\nu = \lim_{s \rightarrow \infty} \phi = 1/2. \quad (6b)$$

### B. Anisotropic AFM spin chains with integer spin<sup>3</sup>

The  $O(3)$   $\sigma$  model with anisotropy can be mapped into the large  $s$  limit of integer-spin XXZ chains. It is argued that this mapping indicates a mechanism for generating a mass gap in the anisotropic  $O(3)$   $\sigma$  model via the condensation of vortices of topological charge 1/2 (merons) present in the XY-like phase of the  $\sigma$  model. A vortex is a planar spin configuration, and condensation involves formation of vortex-antivortex bound pairs.

### C. Anisotropic and alternating AFM spin chains with integer spin<sup>4</sup>

By analogy with fractionally charged soliton states in, say, polyacetylene, spin-1/2 soliton states are believed to be associated with alternating antiferromagnetic chains. A close analogy is pointed out between dyons (magnetic monopoles with charge) in grand unified field theories and solitons in anisotropic, alternating chains. Neutron scattering experiments on suitable 1D experimental systems (no appropriate realization is available at present) are proposed.

It appears that usual and unexpected phenomena may occur in a class of systems, Heisenberg-like spin chains, whose behavior was previously thought to be qualitatively well known and unremarkable.<sup>9</sup> Since the Heisenberg spin chain can be reasonably considered as the simplest realistic model of magnetism, the Haldane prediction, if verified, could have far-reaching consequences for the field of magnetism. For example, the Haldane mapping is not restricted to 1D: the possibility remains of unusual critical behavior also

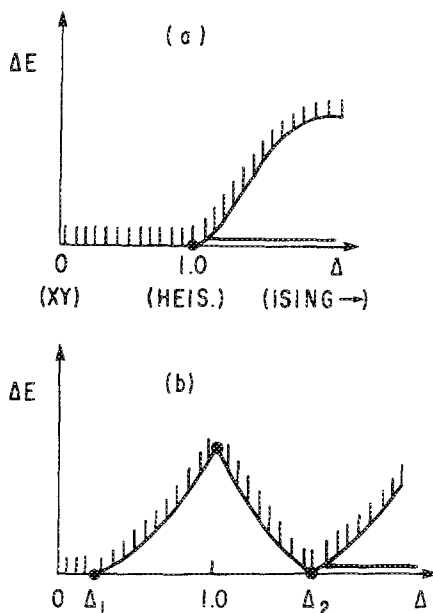


FIG. 1. Schematic plot of the Haldane prediction for (a) half-integer and (b) integer spin XXZ chains.

in higher- $D$  systems.<sup>1</sup> Furthermore, the various predictions point to a richness of  $T = 0$  critical behavior which makes the study of these systems a most interesting and challenging problem in basic statistical mechanics. Hence it is of considerable interest and importance to verify the extent of the validity of the Haldane and Affleck mappings. The interesting feature of these higher-spin quantum chains is that, unlike the familiar case of the spin-1/2  $XXZ$  chain, they are, in general, believed to be nonintegrable (i.e., no exact analytic solution is possible). Therefore, the investigation must perforce rely on approximate numerical techniques, and considerable care must be exercised to avoid misleading conclusions. Results so far indicate a surprising richness of phase behavior and some puzzling aspects of the spectrum of low-lying excitations. We should consider the possibility that some of the unusual phenomena observed are precursors of chaotic behavior expected in nonintegrable quantum systems in the thermodynamic limit.<sup>10,11</sup>

The appropriate way to approach the general quantum spin chain problem would be to start with the basic Heisenberg AFM Hamiltonian [Eq. (1)] and add various symmetry-breaking perturbations. Hamiltonians (2) and (3) show the effect of adding (1) alternation and (2) spin anisotropy. Other perturbing terms which have added include (3) single-ion anisotropy:

$$H = J \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1} + D \sum_{i=1}^N (S_i^z)^2; \quad (7)$$

(4) biquadratic (and higher-order multipolar) exchange

$$H = J \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta \sum_{i=1}^N (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2; \quad (8)$$

and (5) a magnetic field:

$$H = J \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1} - g\mu_B H \sum_{i=1}^N S_i^z. \quad (9)$$

Note that perturbations (7) and (8) are trivial constants in the case of spin-1/2. The five different terms which can be added to the basic Heisenberg Hamiltonian (for  $s > 1/2$ ) generate a multiparameter space expected to be rich in conventional critical phenomena such as first-order transitions, multicritical points, and order (disorder) trajectories. In addition, we expect to observe spectral behavior characteristic of nonintegrable systems.

## THE HALDANE PREDICTION

The predictions of Haldane are expected to be most easily observable in the case of spin-1, according to the gap equation (4), and spin-1 chains have received the bulk of present attention. The considerable amount of numerical work includes finite chain,<sup>12-14</sup> finite-size scaling,<sup>13,15-18</sup> variational,<sup>18,19</sup> Monte Carlo,<sup>20,21</sup> and other calculations.<sup>22-28</sup> Let us first consider evidence pertaining to predictions for the spin-1  $XXZ$  chain described by Hamiltonian (3), as shown schematically in Fig. 1(b). The present consensus is that the weight of numerical evidence supports the prediction, although some puzzling features remain. Enlarging the parameter space of the Heisenberg Hamiltonian (1) by inclusion of single-ion anisotropy [Eq. (7)] in addition to  $XXZ$  anisotropy [Eq. (3)] yields the complicated phase diagram

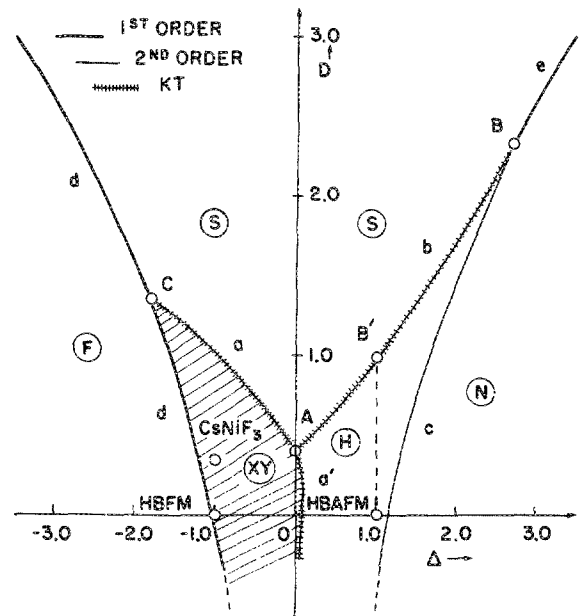


FIG. 2. Phase diagram for  $s = 1$   $XXZ$  chains with single-ion anisotropy, drawn in accordance with existing calculations.

of Fig. 2, representing a consensus of most numerical approaches. Figure 2, discussed in detail below, supports and illuminates features observed for the  $XXZ$  model alone.

It has taken time to reach a consensus because early observations resulted in controversy. These observations<sup>12,18</sup> concerned the fact that when the same numerical approaches, primarily finite-size scaling analyses, which claimed to unambiguously validate Haldane's prediction, were tested on the exactly solvable  $spin-1/2$   $XXZ$  model, qualitatively similar phenomena were observed. The observations in the spin-1/2 case were known rigorously to be incorrect, suggesting much greater caution in numerical analysis. It has been subsequently rather definitively established, however, that spin-1/2 and spin-1 systems are intrinsically dissimilar.

In the region of planar anisotropy  $0 \leq \Delta < 1$ , two main approximate numerical methods have been used: finite-size scaling calculations,<sup>13,15-18</sup> and calculations focusing on obtaining the correlation function exponent  $\eta_x$ .<sup>15-18,23-25</sup> The different methods<sup>28</sup> consistently predict that  $\Delta_1$  exists, and is located in the vicinity of the  $XY$  limit, i.e.,  $0 < \Delta_1 < 0.2-0.3$  as sketched in Fig. 2. The situation in the region of uniaxial anisotropy,  $\Delta > 1$ , is more complex. The prediction that a critical value of  $\Delta$  ( $\Delta_2$ ) exists is supported by most numerical approaches which agree on a numerical value of  $\Delta_2 \sim 1.18-1.20$ , shown on Fig. 2. However,  $\Delta_2$  is determined by the closing of the gap between the  $S_T^z = 0$  ground state and the  $S_T^z = 0$  first excited state. The Haldane prediction implies that an entire quasidegenerate continuum should develop at the critical point  $\Delta_2$ , and that the critical exponents should be Ising-like. Calculations of the correlation function exponent  $\eta_z$  (Refs. 15 and 18) give a value very close to the predicted  $\eta_z = 1/4$ . Furthermore, the integrated intensity

$$I^z(q) = \sum_{i=1}^N e^{-iqR} \langle S_i^z S_{i+1}^z \rangle$$

calculated numerically as a function of  $\Delta$  in the region near  $k = \pi$  shows a compelling resemblance to the equivalent quantity<sup>28</sup> for the spin-1/2 transverse Ising model, justifying the mapping, and indicating a second-order critical point at  $\Delta_2 \sim 1.20$ .

Let us now turn to a discussion of the situation at the Heisenberg point,  $\Delta = 1$ , where the Haldane gap is predicted to be maximal. We discuss the variety of numerical methods available or developed in order to investigate the situation in some detail. Early evidence for a gap came from finite-size scaling calculations on spin-1 chains,<sup>15,16</sup> followed by extrapolations of the quantity  $N\Delta E$  (scaled gap)<sup>12,13</sup> which appeared to diverge instead of converging to a finite value, as is the case for the spin-1/2 chain. Direct plots of  $\Delta E$  vs  $N^{-1}$  up to  $N = 10$  predicted a gap  $\Delta E/J \sim 0.23$ <sup>16</sup> on extrapolation to  $N \rightarrow \infty$ . Subsequent extrapolations on chains up to 14 spins taking account of the curvature of the  $N^{-1}$  plot indicated a higher value  $\Delta E/J \geq 0.35$ .<sup>28</sup> Additional supporting evidence for a gap comes from step ratios associated with the low field behavior of the  $T = 0$  magnetization isotherms, well known to be step functions for finite  $N$ ,<sup>29</sup> and from the behavior of the  $T = 0$  longitudinal integrated intensity  $I^z(\pi)$  which would be divergent for a gapless system but which, in fact, shows a trend that may lead to a finite, non-zero value for  $N \rightarrow \infty$ .<sup>29</sup> However, the most direct and most striking evidence for the presence of a Haldane gap comes from quantum Monte Carlo calculations of the lowest states of the spin-1 Heisenberg systems; the ground state ( $S_T = 0$ ) and the two lowest excited states ( $S_T = 1$  and  $2$ ).<sup>29,30</sup> The Monte Carlo data, together with finite-chain data for  $s = 1$ , convincingly indicate the presence of a gap, even allowing for residual statistical uncertainty. Note that the Monte Carlo data extend out to  $N = 32$ , in conformity with an early observation based on the large- $N$  behavior of the spin-1/2 chain that chain lengths of  $N \geq 25$  may be required to give an accurate quantitative prediction of the asymptotic large  $N$  behavior.<sup>12</sup> The gap value indicated by the Monte Carlo data is  $\Delta E/J \sim 0.41$ , which is quite large, large enough to be experimentally observable.

It is an "act of faith" among those who use finite-size scaling and other numerical techniques that the properties of the system in the thermodynamic limit are governed by the lowest excitations for finite  $N$ . This is certainly the case for all finite  $N$  calculations on integrable systems thus far studied. It is not guaranteed that this is always the case for nonintegrable systems. In fact, an example has been found where the lowest-lying excitation which is a triplet for small  $N$  becomes a singlet for larger  $N$ .<sup>11,31</sup> Therefore, the low-lying spectral excitations of the spin-1 Heisenberg AFM chain have been studied as a function of  $S_T^z$  ( $S_T$ ) and wave-vector  $k$  for spin-1 Heisenberg chains up to  $N = 14$  spins.<sup>14,32</sup> The ground state is always a singlet at  $k = 0$  and the first excited state is the much-studied triplet at  $k = \pi$ , one member of a branch of triplet states for general  $k$  analogous to the des Cloizeaux-Pearson triplets for spin-1/2. The gap between the ground state and the triplet state at  $k = 2\pi/N$ , i.e., essentially the gap behavior at the zone center as opposed to the behavior at the zone boundary, has been studied and appears to converge rather smoothly to a value close to that of the

primary gap at  $\pi$ .<sup>28,33</sup> However, interesting modes with  $S_T = 0, 1, 2, \dots$  have been observed which seem to have the propensity for becoming "supersoft," i.e., degenerate as  $N \rightarrow \infty$  with the ground state of the entire system rather than with the lowest state of their particular  $S_T$  continuum (soft modes). Extrapolated versus  $N^{-1}$ , these states tend smoothly to values *below* the singlet-triplet "primary" gap  $\Delta E/J \sim 0.41$ , perhaps even to zero.<sup>32</sup> It is the case that these are states of intermediate  $k$  which customarily show enhanced finite-size effects. Nevertheless, further investigation of this class of states, possibly by quantum Monte Carlo techniques, seems indicated since they have the potential for radically modifying the Haldane picture.

The early controversy and residual uncertainties point to the importance of experimental investigation of the Haldane prediction, i.e., the existence and magnitude of the gap. Two available candidates for study are cesium nickel trichloride  $\text{CsNiCl}_3$  and rubidium nickel trichloride  $\text{RbNiCl}_3$ . So far, experimental work has appeared only on  $\text{CsNiCl}_3$ ,<sup>34</sup> which is an easy-axis effective spin-1 Heisenberg AFM system in which the  $\text{Ni}^{2+}$  ions form chains parallel to the  $c$  axis of the hexagonal lattice. Neutron scattering studies reveal the presence of a gap above the 3D ordering temperature whose magnitude is equal to, or even greater than, the theoretically predicted value. However, this is not a simple system in that two 3D phase transitions have been observed in the ordered phase. Values of the single-ion parameter  $D$  and interchain coupling obtained (using spin-wave theory) in the 3D ordered phase differ considerably from results obtained in earlier studies. As we shall shortly see, the Haldane gap is sensitive to parameters like the single-ion anisotropy  $D$ . In fact, it is surprising that 3D ordering is observed at all in zero field in a system with such a relatively large gap. The system copper nitrate,  $\text{Cu}(\text{NO}_3)_2 \cdot 2.5\text{H}_2\text{O}$  (Refs. 35 and 36) is a spin-1/2 alternating system with a relatively large gap  $\Delta E/J \sim 5$  K, corresponding to alternation parameter  $\delta \sim 0.57$ . (Recall from above that *uniform* spin-1 chains are predicted to behave like *alternating* spin-1/2 chains.) In the copper nitrate system, ordering is not observed in zero field but between upper and lower critical fields  $H_{c1}$  and  $H_{c2}$ . (For copper nitrate,  $H_{c1} \sim 29$  kOe and  $H_{c2} \sim 45$  kOe.) For the  $\text{CsNiCl}_3$  system,  $J \sim 26$  K and hence the critical field at which quasi-1D (3D) ordering is expected to set in is  $\sim 90$  kOe. It appears worthwhile to develop other Haldane systems of simpler structure than  $\text{CsNiCl}_3$ .

## GENERAL PHASE DIAGRAM

We now turn to the interesting phase behavior observed as a result of numerical approaches, mostly finite-size scaling approaches, to the nonintegrable model of a spin-1 Heisenberg Hamiltonian with two additional parameters,  $XXZ$  anisotropy combined with single-ion anisotropy [see Hamiltonians (3) and (7)]. There is a consensus<sup>37</sup> that for  $D \geq 0$ , the phase diagram has the following features of interest, shown schematically in Fig. 2. For  $\Delta < 0$ , the model has ferromagnetic (FM) character. Line ( $d$ ) passing through the FM Heisenberg point represents a line of first-order transitions to a FM ordered phase (denoted  $F$ ). The line ( $a'$ ) is a line of Kosterlitz-Thouless (KT) transitions terminating a



gapless  $XY$ -like or  $KT$  phase region (denoted  $XY$ ). There is currently an unresolved question whether the portion of the boundary line ( $a'$ ) is as shown, or is coincident with the  $D$  axis. Point  $C$  is a multicritical point where line ( $a$ ) joins the first-order line ( $d$ ). The region  $S$  is a nonordered phase with singlet ground state and an excitation gap characteristic of systems with (large) positive single-ion anisotropy. All methods give consistent qualitative results for the FM portion of Fig. 2. The AFM ( $\Delta > 0$ ) portion has been more difficult to determine and hence has been more controversial. A number of unusual features apparently occur. Line ( $c$ ) has Ising-like character, separating a region with nonordered singlet ground state and excitation energy gap (denoted  $H$ ) from a region ( $N$ ) with doubly degenerate ground state and antiferromagnetic long-range order, frequently referred to as the Néel phase,  $N$ . Since the Heisenberg AFM point is situated within the novel  $H$  phase, the phase is commonly referred to as the "Heisenberg" phase. The distinction between the singlet phase  $H$  and the singlet phase  $S$  induced by single-ion anisotropy is not at present well defined. The two phases are believed to be separated by a special line ( $b$ ), extending from point  $A$  on the  $\Delta = 0$  axis to the multicritical point  $B$  at the termination of the critical line ( $c$ ). The line ( $b$ ) has  $XY$  character with continuously varying exponents.<sup>38</sup> Line ( $e$ ), the large  $D$  continuation of the Ising line ( $c$ ), is found to be a first-order line, and point  $B$  is a multicritical point at which this first-order line bifurcates into  $XY$  line ( $b$ ) and Ising line ( $c$ ). We shall not discuss the portion of the phase diagram corresponding to  $D < 0$ . A striking aspect of the phase diagram of Fig. 2 is the difference from the phase diagram of the same model treated in a variational (mean-field) approach. The mean-field phase diagram is (a) symmetric about the  $D$  axis and (b) shows no Heisenberg phase.<sup>18</sup> No Heisenberg phase is observed in a spin-wave approach either.

Quantitative values can be assigned to features of the phase diagram. In the FM portion of the phase diagram, line ( $d$ ) asymptotically approaches the value  $D = -\Delta$  for large  $D$ . Line ( $a'a$ ) is found numerically to have the exponent value  $\eta \sim 0.25$ , characteristic of the boundary of a  $KT$  phase region. The multicritical point  $C$  is characterized by the values  $(D, \Delta) \sim (1.35, -1.8)$ .<sup>13,17</sup> Note that the experimental system  $\text{CsNiF}_3$ , a planar spin-1 ferromagnet much studied in the context of sine Gordon solitons, is thought to be characterized by the values  $(0.38, -1)$  and hence has critical exponent  $\eta \sim 0.1$ ,<sup>17,18</sup> in agreement with neutron scattering experiments.<sup>39</sup> Point  $A$  has the values  $(0, \sim 0.4)$ .<sup>16,17</sup> In the AFM portion, line ( $e$ ) tends to be the asymptotic value  $D = +\Delta$  for large  $D$ . The multicritical point  $B$  has the values  $(2.3-2.4, 2.75-2.6)$ .<sup>16,17,23</sup> Along line ( $b$ ),  $\eta$  varies from  $\sim 0.25$  at  $A$  to  $\sim 0.67$  at  $B$ .<sup>17,23</sup> Finally, the  $\Delta$  axis cuts line ( $d$ ) at  $(0, -1)$  and line ( $c$ ) at  $(1, 1.8-1.20)$ .<sup>15,16</sup>

The phase diagram of Fig. 2 shows an interesting new effect. Consider the behavior of the system along the line  $\Delta = 1$ ,  $D > 0$ . Simple spin-wave theory predicts that for  $D > 0$ , a gap opens up away from the (gapless) Heisenberg point linearly in  $D$ , i.e.,  $\Delta E \propto D$ . According to the variational calculation,<sup>18</sup> the system remains gapless out to a critical  $D_c$ , and then a gap opens proportional to  $D$ . From Fig. 2, how-

ever, it follows that the gap must decrease with increasing  $D$  out to the gapless point  $B'$  on line ( $b$ ), where  $B'$  has the values  $(\sim 1.0, 1.0)$ ,<sup>16</sup> and then a gap opens up again in the singlet phase for  $D > 1$ . The Haldane prediction implies that the behavior of an AFM effective spin-1 system with exchange and single-ion anisotropy is far more complex than previously realized, and that experimental analyses should proceed with caution.

## THE AFFLECK PREDICTIONS

The validity of the Haldane prediction for the spin-1 quantum chain appears to have been as convincingly established as current numerical methods allow. Specifically, it has been established that low-lying classes of excitations are present which conform to Haldane's prediction. The question remaining is whether other excitation classes occur in addition (e.g., supersoft modes<sup>32</sup>) showing different behavior which become important closer to the thermodynamic limit. Evidence for the validity of Affleck's predictions, which are more recent, is not so convincing. However, numerical work has only just begun.

Recent developments in the theory of conformal invariance have been directed towards identifying the value of the conformal anomaly  $c$  (central charge of the Virasoro algebra) for a particular integrable model,<sup>40,41</sup> and predicting values for the associated critical exponents. For example, in 1D, the value  $c = 1/2$  corresponds to the spin-1/2 anisotropic  $XY$  model at its critical field, and the value  $c = 1$  to the spin-1/2  $XXZ$  model with planar anisotropy.<sup>40,41</sup> Recently the Russian schools in Moscow and Leningrad have discovered a Bethe Ansatz integrable class of AFM-like models of higher spin.<sup>42,43</sup> The Hamiltonians for this class take the form of an expansion in powers of  $(\mathbf{S}_i \cdot \mathbf{S}_{i+1})$  of degree  $2s$ . For example, Hamiltonian (8) with  $\beta = 1$  is the spin-1 member of the class, and the familiar spin-1/2 AFM Heisenberg model is the spin-1/2 limiting member. The  $c$  values are given by<sup>41</sup>

$$c = 3s/(1+s), \quad (10)$$

i.e., this is a class of  $c > 1$  models, and the  $s$  dependence means that each model is in a different universality class. The  $s$  dependence appears also in the critical exponents: for example, the prediction for the exponent  $\eta$  is<sup>2</sup>

$$\eta = 3/2(1+s). \quad (11)$$

For  $s = 1/2$ , the value for  $\eta$  is found to be  $\eta \sim 0.87$  (Refs. 23 and 24) from a variety of approximate numerical approaches,<sup>44</sup> in fair agreement with the predicted value  $\eta = 1$ . For spin-1, the value  $\eta \sim 0.65-0.67$  obtained numerically<sup>45</sup> is in reasonable agreement with the predicted value  $\eta = 3/4$ . Hence, although agreement is only to within about 13% in each case, the numerical studies do appear to confirm the predicted  $s$  dependence of  $\eta$ .

Affleck<sup>2</sup> predicts that the following perturbations applied to the gapless spin-1 Russian model [Hamiltonian (8) with  $\beta = 1$ ] induce a gap:  $xxz$  anisotropy (gap exponent = 1); biquadratic exchange [gap exponent = 0.615; see Eq. (2) with  $s = 1$ ]. Finite-size scaling investigations<sup>31,44,45</sup> are generally in poor agreement with these pre-



dictions. However, the presence of logarithmic corrections could resolve the discrepancies.

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- <sup>1</sup>F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983), and private communication.  
<sup>2</sup>I. Affleck, Nucl. Phys. B **265**, 409 (1986).  
<sup>3</sup>I. Affleck, Phys. Rev. Lett. **56**, 408 (1986).  
<sup>4</sup>I. Affleck, Phys. Rev. Lett. **57**, 1048 (1986).  
<sup>5</sup>See, for example, R. Kubo, Phys. Rev. **87**, 568 (1952).  
<sup>6</sup>The Haldane prediction does not apply to Heisenberg FM systems which are generically similar for all spin and gapless.  
<sup>7</sup>J. W. Bray, I. S. Jacobs, L. V. Interrante, and J. C. Bonner, in *Extended Linear Chain Compounds* edited by Joel S. Miller (Plenum, New York, 1982), Vol. 3, p. 353.  
<sup>8</sup>The fact that the Haldane phenomenon is apparent in spin chains with  $s$  as low as 1 may relate to a recent observation by Parkinson and Bonner (Ref. 14) that chains with  $s > 1$  show classical behavior at low fields, in contrast to the case of  $s = 1/2$ .  
<sup>9</sup>H. W. J. Blöte, Physica **93B**, 93 (1975). Blöte observed unusual features of the ground state energy and low  $T$  specific heat whose significance was not appreciated at the time.  
<sup>10</sup>G. Müller, Phys. Rev. A **34**, 3345 (1986).  
<sup>11</sup>G. Müller, J. C. Bonner, and J. B. Parkinson (these proceedings).  
<sup>12</sup>J. C. Bonner and G. Müller, Phys. Rev. B **29**, 5216 (1984).  
<sup>13</sup>M. Kolb, R. Botet, and R. Jullien, J. Phys. A **16**, L673 (1983).

- <sup>14</sup>J. B. Parkinson and J. C. Bonner, Phys. Rev. B **32**, 4703 (1985).  
<sup>15</sup>R. Botet and R. Jullien, Phys. Rev. B **27**, 613 (1983).  
<sup>16</sup>R. Botet and R. Jullien, and M. Kolb, Phys. Rev. B **28**, 3914 (1983).  
<sup>17</sup>U. Glaus and T. Schneider, Phys. Rev. B **30**, 215 (1984).  
<sup>18</sup>J. Sólyom and T. A. L. Ziman, Phys. Rev. B **30**, 3980 (1984).  
<sup>19</sup>J. Sólyom, Phys. Rev. B **32**, 7524 (1985).  
<sup>20</sup>M. P. Nightingale and H. W. J. Blöte, Phys. Rev. B **33**, 659 (1986).  
<sup>21</sup>K. Sogo and N. Uchinami, J. Phys. A **19**, 493 (1986).  
<sup>22</sup>S. -T. Chui and K. B. Ma, Phys. Rev. B **29**, 1287 (1984).  
<sup>23</sup>H. Schulz and T. A. L. Ziman, Phys. Rev. B **33**, 6545 (1986).  
<sup>24</sup>K. Kubo and S. Takada, J. Phys. Soc. Jpn. **55**, 438 (1986).  
<sup>25</sup>H. Nishimori, Prog. Theor. Phys. **73**, 1577 (1985).  
<sup>26</sup>J. Timonen and J. Sólyom (in press).  
<sup>27</sup>U. Glaus (in press).  
<sup>28</sup>A detailed review is presented in J. C. Bonner, J. B. Parkinson, and G. Müller (unpublished work).  
<sup>29</sup>J. B. Parkinson, J. C. Bonner, G. Müller, M. P. Nightingale, and H. W. J. Blöte, J. Appl. Phys. **57**, 3319 (1985).  
<sup>30</sup>M. P. Nightingale and H. W. J. Blöte, Phys. Rev. B **33**, 659 (1986).  
<sup>31</sup>J. C. Bonner, J. B. Parkinson, J. Oitmaa, and H. W. J. Blöte (these proceedings).  
<sup>32</sup>J. C. Bonner and J. B. Parkinson (unpublished work).  
<sup>33</sup>An examination of other prominent low-lying modes is to be found in Ref. 14. These modes have a gap in the thermodynamic limit.  
<sup>34</sup>W. J. L. Buyers, R. M. Morra, R. L. Armstrong, M. J. Hogan, P. Gerlach and K. Hirakawa, Phys. Rev. Lett. **56**, 371 (1986). See also M. Steiner, K. Kakurai, and J. K. Kjems (these proceedings).  
<sup>35</sup>J. C. Bonner, S. A. Friedberg, H. Kobayashi, D. L. Meier, and H. W. J. Blöte, Phys. Rev. B **27**, 248 (1983).  
<sup>36</sup>M. Diederix, H. W. J. Blöte, J. P. Groen, T. O. Klaassen, and N. J. Poulis, Phys. Rev. B **19**, 420 (1979).  
<sup>37</sup>The authors of Ref. 18 obtain substantially similar numerical results for  $N$  up to 8 as other workers, but differ from the consensus in their interpretation.  
<sup>38</sup>A calculation on a classical spin-1 classical rotator model with spin anisotropy and single-ion anisotropy [D. C. Mattis, Phys. Rev. B **31**, 4698 (1983)] is interesting in connection with Fig. 2.  
<sup>39</sup>J. K. Kjems, K. Kakurai, and M. Steiner, J. Magn. Magn. Mater. **32-34**, 1133 (1981).  
<sup>40</sup>H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986).  
<sup>41</sup>I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).  
<sup>42</sup>L. A. Takhtajan, Phys. Lett. **87A**, 479 (1982).  
<sup>43</sup>H. M. Babujian, Phys. Lett. **90A**, 479 (1982).  
<sup>44</sup>Note that the Bethe Ansatz approach allows an analytic calculation of the thermodynamic properties, but not the correlation functions.  
<sup>45</sup>J. Oitmaa, J. B. Parkinson, and J. C. Bonner, J. Phys. C **19**, L595 (1986).  
<sup>46</sup>H. W. J. Blöte and H. Capel, Physica A (in press).