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Excitations and Critical Behavior in Generalized Heisenberg Spin Chains

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1. Introduction

Heisenberg spin chains which represent the simplest realistic models for magnetic insulators were thought to be well understood and generically similar for any spin-value s. This is expressed in the spin-wave approach to Heisenberg spin chains [1]. Consequently surprise and some degree of controversy resulted from recent work of Haldane [2,3], who proposed a dramatically different picture. Consider the spin-s XXZ Hamiltonian with anisotropy parameter Δ:

$$H = J \sum_{l=1}^{N} \left\{ S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z \right\}. \tag{1}$$

For half-integer s, the region $0 \leq \Delta < 1$ is a gapless phase with power-law decay of the two-spin correlation functions, terminating in an essential singularity at $\Delta = 1$. For $\Delta > 1$, the ground state consists of two degenerate singlet states associated with long-range order and a gap to an excitation continuum. For integer s, on the other hand, the gapless phase associated with planar anisotropy extends only over a range $0 \leq \Delta \leq \Delta_1$ ($\Delta_1 < 1$) and the phase with gap and ordered ground state extends over $\Delta \geq \Delta_2$ ($\Delta_2 > 1$). A new phase (called hereafter the Haldane phase) appears in the region $\Delta_1 < \Delta < \Delta_2$ encompassing the Heisenberg point at $\Delta = 1$. The Haldane phase ground state is a non-ordered singlet with exponentially decaying spin correlation functions, and there is a gap to an excitation continuum, which has its maximum value at $\Delta = 1$. The spin-dependent gap at $\Delta = 1$ is given by $\Delta E/J \sim s^2 \exp(-\pi s)$.

Generalized Heisenberg spin chains are not exactly solvable (Bethe Ansatz integrable) for $s > 1/2$, except in very special situations. Hence Haldane's conjecture has, perforce, been investigated with a variety of numerical techniques, including scaled-gap and finite-size scaling calculations, finite-chain extrapolations, variational approaches and various correlation function calculations [4]. Obtaining reliable numerical results turns out to be quite difficult and great care must be taken. For example, while the first numerical, finite-size scaling calculation on spin-1 XXZ chains [5] revealed the predicted Haldane phenomena, it was subsequently demonstrated that a "pseudo-Haldane picture" is obtained also for the spin-$1/2$ XXZ model [6] in contradiction to exact analytic results. However, it is now the consensus of a large body of numerical work that the Haldane picture is, nevertheless, correct, and experimental support for this conclusion is starting to appear [7].

On the basis of a comprehensive numerical study and survey we have concluded that the various classes of excitations predicted by Haldane for the spin-1 model are all present and behave as conjectured [8]. However, we observe additional interesting features, in particular, classes of excitations which have the potential for modifying somewhat the basic Haldane picture, as we will discuss.

The addition to the basic Heisenberg Hamiltonian of exchange anisotropy, single-ion anisotropy, biquadratic exchange, or a magnetic field, generates a rich and complicated phase diagram for chains with s $> 1/2$ [4]. Unusual spectral features in generalized spin-1 chains will be discussed in the context of nonintegrability effects and quantum chaos [9,10].

2. Spin-1 Heisenberg Antiferromagnetic Chain

Since the predicted singlet-triplet Haldane gap is a maximum at the isotropic Heisenberg point, $\Delta = 1.0$, numerical attention has focussed on this limit. While several numerical techniques have been devised to study this problem [8], the most direct approach is to examine the behavior of the Haldane gap for a sequence of finite systems of increasing size and examine the trend as $N \to \infty$. Fig. 1 shows finite-N gaps for up to $N = 20$ spins with $s = 1/2$ as a function of $1/N$. The gaps extrapolate convincingly to a value very close to zero, in agreement with the exact result that this system should be gapless in the limit $N \to \infty$. Exact results up to $N = 14$ for the $s = 1$ case, on the other hand, show concave upwards curvature, consistent with a nonzero gap in the limit $N \to \infty$. However, since earlier studies [6] have pointed to the importance of obtaining data for very long chains to be sure of observing a reliable large N trend, a quantum Monte Carlo approach was developed to obtain data out to $N = 32$ spins [11]. The Monte Carlo data continue the concave upward trend of the exact finite-N data and predict a limiting singlet-triplet gap of magnitude

$$\Delta E/J \sim 0.41. \tag{2}$$

This gap occurs at the Brillouin zone boundary, since the excited triplet is at $k = \pi$ and the ground state is always a $k = 0$ state. The Haldane conjecture implies that a gap of equal magnitude should occur at the zone center. In Fig. 1, the finite-N triplet gaps for the $k = 2\pi/N$ mode are shown, for $N \leq 14$. The convergence is quite regular, and the extrapolated limit is in reasonable agreement with Eq. (2).

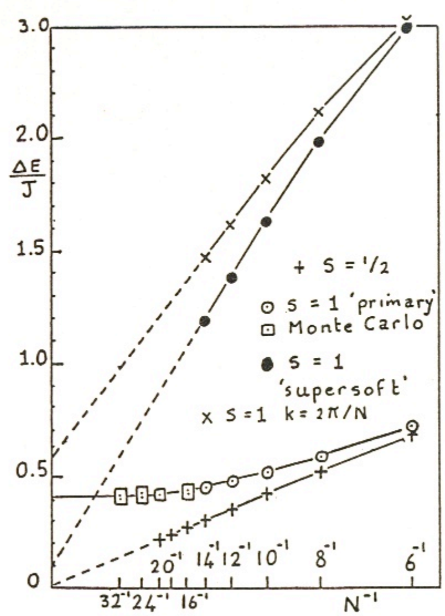

Figure 1. Various excited modes for the $s = 1$ antiferromagnetic Heisenberg chain as discussed in the text.

There does, however, appear to be one remarkable feature associated with the spectral excitations in the Heisenberg limit and vicinity. Numerical studies have revealed a crossover in the character of the spectral excitations as a function of field [12]. At high fields, the low-lying dispersion spectra are qualitatively similar to those for $s = 1/2$, i.e. have quantum character. At low fields, on the other hand, the dispersion spectra display notable classical character, with one complication. An additional set of modes occurs which appears unrelated to the classical spectra. When extrapolated as a function of $1/N$, these anomalous modes project *below* all other excitations with the same value of S_T^z. For this reason these states have been termed"supersoft" modes

[12]. In particular the $S^z_T = 1$ mode lies at $k = \pi/N$, and its excitation energy is included in Fig. 1. Extrapolating below all other excited states it appears to extrapolate below the triplet at $k = \pi$ which has been used to determine the Haldane gap! The curvature is consistently concave downwards and increases with increasing N, making it unlikely that the curve could develop an inflection point for larger N and tend to the value (2).

Detailed information on the $T = 0$ phase behavior of quantum spin chains may be inferred from the integrated intensity

$$I(k) = \sum_{R=-\infty}^{+\infty} e^{ikR} \langle \vec{S}_l \cdot \vec{S}_{l+R} \rangle. \tag{3}$$

At zero temperature, $I(k)$ is a property of the ground state solely, and yet also contains information on the excited states, at wave number k. It can be shown [8] that in the presence of a gap ΔE between the ground state and the lower edge of the excitation continuum, the integrated intensity must satisfy the following inequality:

$$I(k) \leq 2|E_G|(1 - \cos k)/3\Delta E, \tag{4}$$

where E_G is the ground-state energy per spin. For the Heisenberg spin-1 chain calculations of Blöte and Nightingale [11] give $E_G/J \sim -1.4015$. Together with (3) this yields the following lower bound for the inverse integrated intensity: $I^{-1}(\pi) \geq 0.219$. A plot of $1/I(\pi)$ versus $1/N$ is consistent with this bound in the limit $N \to \infty$, but a plot of the inverse intensity $1/I(\pi - 2\pi/N)$, which is dominated by the $S^z_T = 1$ supersoft mode, fails appreciably to satisfy this criterion and is not consistent with an energy gap (2).

Hence present numerical evidence out to $N - 16$ spins is consistent with the presence of a special class of excitations not predicted by Haldane. These isolated excitations probably have insufficient thermodynamic weight to affect the thermal properties, but since there exist $N/2$ such modes (corresponding to $S^z_T = 1, 2, \ldots, N/2$), they should be experimentally observable in the $T = 0$ magnetization isotherm at low magnetic fields. In particular, the $T = 0$ magnetization isotherm should become zero at a much lower field than that corresponding to the Haldane gap (2).

3. Spin-1 XXZ Model

Of all the excitation phenomena predicted by Haldane to occur for the $s = 1$ XXZ model, the one which is most difficult to confirm numerically has been the behavior in the vicinity of the critical point Δ_2 [13]. In fact, doubt has even been expressed concerning the validity of this particular aspect of the conjecture. Haldane predicts that the transition at $\Delta = \Delta_2$ should be in the universality class of the spin-1/2 transverse Ising model. It has already been established [4,8] that at $\Delta_2 \sim 1.18 - 1.20$, the Haldane gap disappears and an excited $S^z_T = 0$ state becomes degenerate with the $S^z_T = 0$ ground state for $\Delta > \Delta_2$. The mapping to the transverse Ising model implies the existence in the limit $N \to \infty$ of an infinite continuum of scaling states quasi-degenerate with the ground state (states) at, and only at, $\Delta = \Delta_2$. The development of this scaling continuum is not very apparent in the spectra for small finite systems. A search for the scaling states implied by the Haldane conjecture revealed a class of high-lying $S^z_T = 0$ excitations at $k = 0$. Plotted as a function of Δ, these excitations are shown in Fig. 2. A minimum develops in the vicinity of $\Delta \sim 1.1 - 1.2$ which intensifies with increasing N. Fitting a polynomial through data in the vicinity of the minimum and plotting the excitation gap at the polynomial minimum versus $1/N$ yields an extrapolated value well below the lower edge of the triplet ($S^z_T = 1$) continuum, and even consistent with a value zero. We conclude these are the Haldane scaling states at Δ_2. This conclusion is reinforced by a detailed study of corresponding excitations for the spin-1/2 transverse Ising model near the critical field. The transverse Ising model picture shows a striking resemblance to Fig. 2.

A surprising feature of the Haldane prediction [3] is that the zz-correlation function decays as a power law, $|\langle S^z_l S^z_{l+R} \rangle| \sim R^{-1/4}$, whereas the correlation function $\langle S^x_l S^x_{l+R} \rangle$ decays exponentially for $R \to \infty$. This unusual prediction implies that the fluctuations are critical in the longitudinal (z)

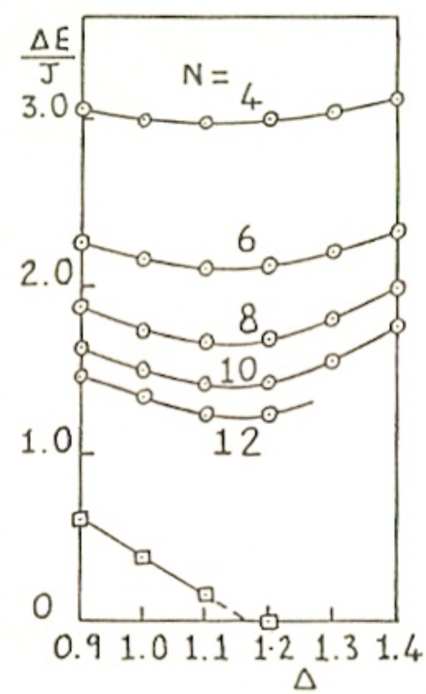

Figure 2. $S_T^z = 0$ "scaling" states for $N = 4, 6, 8, 10$ and 12 (denoted by $\circ$). The excitation denoted by $\square$ is the extrapolated limit of the upper component of the $\Delta \geq \Delta_2$ ground state.

direction but not in the transverse (x) direction. Such a situation has not been observed previously. Hence we examined also the $S_T^z = 1$ excitations at $k = 0$ as a function of Δ, and again observed the development of minima with increasing N in the vicinity of Δ_2. These minima also display a potential for extrapolating to zero, analogous to the $S_T^z = 0$ minima, and in contrast to $k = 0$ excitations in the same class corresponding to $S_T^z = 2$, etc. If gapless $S_T^z = 1$ excitations occur at $\Delta = \Delta_2$, the transverse xx-correlations will also display power-law decay, in disagreement with Haldane's specific predictions for the behavior of the two-spin correlation functions [2].

4. Nonintegrability Aspects of the Spectra

The above numerical studies of the spin-1 XXZ model, including the Heisenberg point, show that the Haldane prediction represents a remarkably successful mapping. All classes of states predicted by Haldane appear to be present and behave generally as predicted. It appears, however, that we have discovered additional classes of states whose presence have the potential of playing an important role in the extended $T = 0$ phase diagram. The $|S_T^z| = 1$ "scaling" states at $\Delta \sim \Delta_2$ are perhaps less surprising since anaIogous states occur for the transverse Ising model near the critical field. The "supersoft" modes at $\Delta = 1$, on the other hand, are a remarkable feature not encountered previously in any integrable model. Here we discuss in more detail the possible occurrence in generalized $s \geq 1$ Heisenberg spin chains of spectral features which are characteristic of nonintegrable models.

Consider the spin-1 Heisenberg antiferromagnetic chain generalized by addition of biquadratic exchange:

$$H/J = \sum_{l=1}^{N} \vec{S}_l \cdot \vec{S}_{l+1} - \beta \sum_{l=1}^{N} \left(\vec{S}_l \cdot \vec{S}_{l+1}\right)^2. \tag{5}$$

Special limits of this bilinear-biquadratic exchange Hamiltonian are:

$\beta = 0$	Heisenberg model	(nonintegrable)
$\beta = 1$	“Russian” model [14]	(integrable)
$\beta = \infty$	pure biquadratic	(nonintegrable)

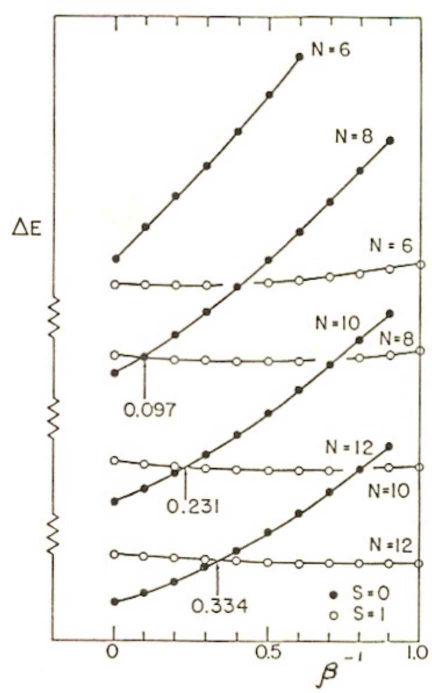

Figure 3. A plot of the values of β^{-1} at which the lowest excited state in the range $0 \le \beta^{-1} \le 1$ changes from a singlet to triplet versus N^{-1}. The rough extrapolated limit of the crossing points is consistent with the value unity, implying that the singlet is ultimately the dominant excited state in this range.

Hamiltonian (8) at the special point $\beta = 1$ is an example of an $s > 1/2$ model which is Bethe Ansatz integrable and gapless [14,15]. Hence it is of interest to investigate the parameter range $0 \le \beta \le \infty$ to determine the extent of the gapless region. A prediction of Affleck [16] is that only the point $\beta = 1$ is gapless and that a gap opens on either side of the Russian point as $\Delta E \sim |1 - \beta|$l. Numerical studies including scaled-gap [17] and other finite-size scaling calculations [18,19] are consistent with Affleck in predicting the opening of a singlet-triplet gap at $\beta = 1$, but differ in predicting that the gap opens up more slowly than linearly. Furthermore, numerical calculations revealed a very curious phenomenon in the Russian-biquadratic regime ($0 \le 1/\beta \le 1$) [18]. This phenomenon is illustrated in Fig. 3. Close to the biquadratic limit, the first excited state is no longer the triplet at $k = \pi$ for sufficiently large N, but instead becomes a singlet at π. A crossover effect occurs in this regime, illustrated in Fig. 3, which implies that as $N \to \infty$, the lowest excited state is a singlet over the whole regime. Traditional finite-size scaling approaches which assume, as an act of faith, that the dominant excited states for small finite N remain the dominant states as as $N \to \infty$, can be seriously misled by a situation such as the above. Just as in the case of the supersoft modes, a new class of important modes appears at sufficiently large N. This triplet-to-singlet crossover phenomenon does not occur for integrable systems (e.g. the spin-1/2 XXZ model), and is presumably a spectral nonintegrability effect.

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