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LETTER TO THE EDITOR

Comparison of ground state properties for odd half-integer and integer spin antiferromagnetic Heisenberg chains

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Abstract. Ground state properties of finite anisotropic antiferromagnetic Heisenberg chains are studied for odd half-integer spins $S=\frac{1}{2},\frac{3}{2}\ldots$ as well as integer spins $S=1,2\ldots.$ Finite size scaling analysis of the results clearly distinguishes the half-integer ($S=\frac{1}{2},\frac{3}{2}$) from the integer ($S=1$) spin situation. It gives strong support to a recent conjecture which postulates that the $T=0$ phase structure is very different in the two cases. According to this idea there exists a new phase between the planar and the antiferromagnetic region, for integer spins only. This phase, which includes the isotropic point, has a finite energy gap and no long range order.

The Heisenberg chain has been studied extensively, being one of a few non-trivial and still soluble quantum models. The ground state properties have been determined exactly for the spin $S=\frac{1}{2}$ case with various anisotropies (Bethe 1938, Yang and Yang 1966, Baxter 1972). For $S>\frac{1}{2}$ the model has not been solved. Large S developments indicate that spin wave theory describes the $T=0$ properties quite well down to $S=\frac{1}{2}$ (Steiner *et al* 1976).

Recently, the interest in such systems has increased as experimentally a number of quasi one-dimensional Heisenberg antiferromagnets have been studied (Kjeins and Steiner 1978, Heilmann *et al* 1978). This has motivated theoretical efforts to extend the known $S=\frac{1}{2}$ results. Attempts have been made to understand the continuum of low-lying excitations better (Faddeev and Takhtajan 1981, Hashimoto 1982) and to solve models with $S>\frac{1}{2}$. A class of Heisenberg systems with more complicated interactions has been solved by Bethe ansatz for any value of S (Sutherland 1975, Takhtajan 1982). But the simple Heisenberg model has resisted an exact solution for $S>\frac{1}{2}$. Estimates of ground state and thermodynamic properties for $S>1$ have been obtained by numerical methods applied to finite chains (Blöte 1975).

A major change in view has been pioneered by Haldane (1982, 1983a, b) on the basis of a treatment in terms of quantum action-angle variables. He contends that the $T=0$ properties for even half-integer spins differ fundamentally from odd half-integer spins. This result has stimulated numerical work by two of the present authors (Botet and Jullien 1983) for $S=1$. The ground state and spectral properties are consistent with the findings by Haldane.

Here, we study spin values from $S=\frac{1}{2}$ to $S=3$ and critically compare the even and odd half-integer spins. The conclusions are that $S=\frac{1}{2},\frac{3}{2}$ are very different from $S=1$,

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while for $S>2$ the results show some qualitative, but little quantitative distinction, in agreement with Haldane's proposal. The phase structure for integer spin has been criticised by Bonner and Müller (1983). They claim that the transitions at $\lambda \neq 1$ contradict general principles of critical phenomena. We believe that two separate transitions are compatible with these ideas. However, symmetry requires that if they coincide, it must be at $\lambda=1$ (figure 1). The essential singularity then masks the other.

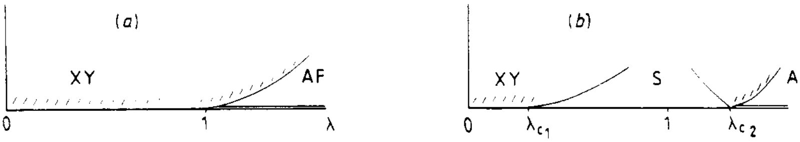

Figure 1. $T=0$ phase structure of anisotropic antiferromagnetic Heisenberg chain. The energy spectrum is sketched as a function of the anisotropy λ. XY, S, AF stand for planar, singlet. Néel doublet phases. (a) Odd half-integer spin, (b) integer spin. Shaded regions indicate a continuum.

Consider the Hamiltonian

$$H_N=\sum_{l=1}^{N}\left(S_{l-1}^{x}S_{l}^{x}+S_{l-1}^{y}S_{l}^{y}+\lambda S_{l-1}^{z}S_{l}^{z}\right)$$

where S_l^x, S_l^y, S_l^z are spin S operators at the N sites of a periodic chain ($\boldsymbol{S}_0 \equiv \boldsymbol{S}_N$). We vary the anisotropy λ from $0<\lambda<1$ (planar) over $\lambda=1$ (isotropic) to $\lambda>1$ (antiferromagnetic). For $S=\frac{1}{2}$ the exact results distinguish between a gapless region (XY phase) with a spin wave spectrum, power-law correlation functions and no long range order and an antiferromagnetic region (AF phase) with a Néel doublet separated by a gap from the excited states and exponential correlations. The transition from XY to AF occurs at the isotropic point, $\lambda=1$, and has an essential singularity. Haldane postulates that this behaviour is characteristic for spins $S=\frac{1}{2}, \frac{3}{2} \ldots$, figure 1($a$). For integer spins $S=1$, 2 (figure 1(b)) there exists a new phase (S phase) intermediate between the XY and the AF regions which has a singlet ground state, a non-zero energy gap and exponential correlation functions. The transition XY–S at $0<\lambda_{c_1}<1$ has an essential singularity. The other transition S–AF at $\lambda_{c_2}>1$ is of the singlet to doublet type. The isotropic Heisenberg chain $\lambda=1$ lies in the S phase. As $S \to \infty$ the difference between integer and odd half-integer spins must disappear. Still according to Haldane, this happens very rapidly with increasing S such that already for the modest values under study this ought to be apparent. Indeed, for $S=2$ the properties differ hardly from half-integer values.

Our approach is complementary to the one by Haldane in the sense that his conclusions are exact when $S \to \infty$ while we work with arbitrary S but finite N. We proceed according to the by now standard method of extrapolating numerically obtained finite N results to $N=\infty$. Finite size scaling and the related phenomenological renormalisation group (PRG) have proven to be useful (Fisher and Barber 1972, Nightingale 1976, Sneddon 1978). The quantities calculated are several energy gaps $g(N, S)=E_x-E_0$ between low-lying excited states and the ground state. Ground state correlation functions and energy derivatives can also be used to analyse the $T=0$ behaviour (Kolb *et al* 1983).

The Hamiltonian H_N has been diagonalised numerically to obtain all low-lying eigenvalues and eigenvectors. To increase the maximum N the symmetries of H_N

have been exploited. They are conservation of total spin along an axis ($\Sigma^z = -N\cdot S, \ldots, N\cdot S$), spin inversion ($F = \pm 1$), left/right symmetry of the chain ($R = \pm 1$) and conservation of the wavevector ($q = (2\pi/N)n$). With reasonable efforts and using the Lanczös method (Whitehead 1980) designed to diagonalise sparsely populated matrices, the largest chains for $S = \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, 3$ are $N = 20, 12, 10, 8, 6, 6$. Only even N are considered, odd N would have to be analysed separately (Blöte 1975). As for $S = \frac{1}{2}$ exact results are available it merely serves to test the convergence as $N \to \infty$.

There is a qualitative distinction between odd half-integer and integer spins. While $\Sigma^z = 0$ for the ground state and $\Sigma^z = 0$ (± 1) for $\lambda > 1$ ($\lambda < 1$) for the lowest excitation independent of S and N, the quantum numbers (F, R, q) for ground state/lowest excitation are $(1, 1, 0)(-1, -1, \pi)$ for integer S and all N but alternate between $(1, 1, 0)/(-1, -1, \pi)$ and $(-1, -1, \pi)/(1, 1, 0)$ for S odd half integer and $\frac{1}{2}N$ even respectively odd. The gaps between ground state and lowest excitation as a function of N and S are shown in figure 2 for $\lambda = 1$ where the distinction between the even and odd half-integer case should be clearest. For $N = 2$, 4 the gap is independent of S. In figure 2(a), the scaled gap grows much more rapidly for $S = 1$ than for $S = \frac{1}{2}, \frac{3}{2}$. Figure 2($b$) illustrates how with increasing N the gap deviates from the spin independent behaviour of $N = 2$, 4 and—for S half integer only—extrapolates to zero. For $S > 2$ the gap deviates so little from the small N (or $S \to \infty$) form that larger N would have to be considered to estimate the asymptotic limit.

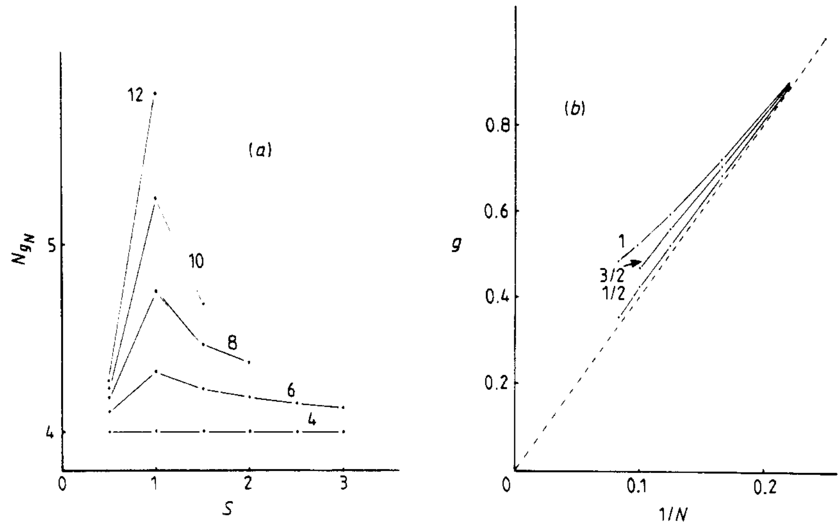

Figure 2. Energy gaps as a function of spin S and number of sites N for the isotropic Heisenberg model ($\lambda = 1$). (a) Scaled gap $Ng(N, S)$ against S with N as parameter. (b) Gap $g(N, S)$ against $1/N$. The labels indicate the spin S. The broken line is the extrapolation of the gaps for $N = 2$, 4 (independent of S). Note that for $S = \frac{1}{2}, \frac{3}{2}$ the gap turns downward, while for $S = 1$ it has an upward trend.

Higher excited states describe the $T = 0$ properties in general less accurately than the first excitation. Nonetheless, they can give useful information. In the integer spin situation, the second gap at the transition λ_{c_2} (figure 1(b)) necessarily has a sharp minimum. A very direct way to determine λ_{c_2} then is to analyse the minimum of this gap. Figure 3 shows $\lambda_{\min}$ (N, S) where the first gap in the subspace of the ground

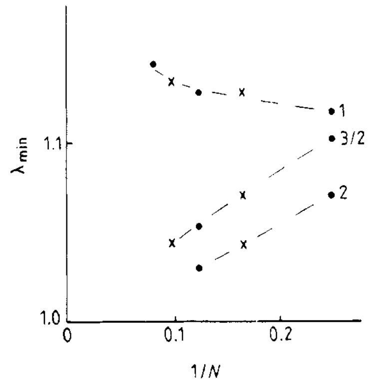

Figure 3. Anisotropy λ_{min} where the gap $g_2(\lambda)$ assumes its minimum against $1/N$ for spins $S=1, \frac{3}{2}, 2 (\partial g_2(\lambda)/\partial\lambda|_{\lambda_{min}}=0)$. g_2 is the gap between the ground state and the first excited state in the same subspace (for $S=\frac{1}{2}$, $g_2(\lambda)$ is practically flat). There are oscillations between $N/2$ even (●) and $N/2$ odd (×).

state has its minimum. For $S=1$ the estimate of λ_{c_2} is at 1.145 for $N=12$ and rising, for $S=\frac{3}{2}$ it tends exactly to 1 from above. For $S=\frac{1}{2}$, $g_2(\lambda)$ is practically constant.

A powerful method to determine a transition is by means of the PRG. Applying it to λ_{c_2}, it gives convincing evidence that half-integer and integer spins are qualitatively different. Defining λ' (λ, N) through $(N+1)g(\lambda, N+1)=(N-1)g(\lambda', N-1)$ we present in figure 4 the estimates $\lambda_c=\lambda'$ (λ_c) for successive values of N. The question of how the results converge as $N\to\infty$ has been considered by Kolb *et al* (1982). The transition for $S=\frac{1}{2}, \frac{3}{2}$ decreases slowly towards $\lambda_c=1$ whereas for $S=1$, λ_{c_2} has a strong upward trend excluding $\lambda_c=1$ as a limiting value. The difference in slope and curvature qualitatively distinguish the points in contradiction to Bonner and Müller (1983). For $S\geqslant 2$ larger values of N are necessary to distinguish the two types of behaviour.

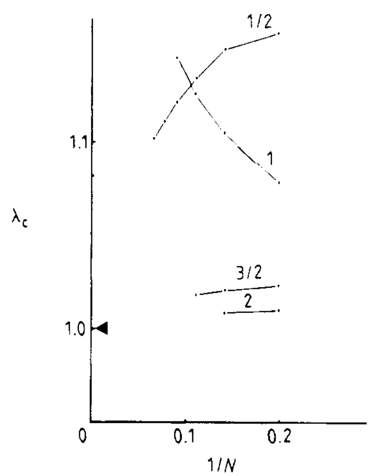

Figure 4. Phenomenological renormalisation analysis for λ_{c_2} $(N+1, N-1)$ against $1/N$ for spins $S=\frac{1}{2}, 1, \frac{3}{2}, 2$.

The other transition λ_{c_1} (figure 1(*b*)) can be investigated by PRG as well. As one expects a line of fixed points λ^*, $0<\lambda^*<\lambda_{c_1}$, $\lambda_c(N)$ provides lower bound for λ_{c_1}. For all S the scaled gaps superimpose in this region.

In conclusion, the comparison of even and odd half-integer spins on finite chains reveals a new phase structure for integer spins. It is most pronounced for the gaps near the isotropic ($\lambda = 1$) model when contrasting $S=\frac{1}{2}, \frac{3}{2}$ with $S=1$. For $S \geqslant 2$, the distinction even/odd is extremely small. The data presented corroborate Haldane's picture. It may be interesting to study the thermodynamic consequences of the new phase. While for $S \geqslant 2$, the effects are probably too small, for $S=1$ the estimated size of the gap at $\lambda=1$ is large enough to be observable.

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