Critical Behavior of the $S = 3/2$ Antiferromagnetic Heisenberg Chain

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Using the density-matrix renormalization-group technique we study the long-wavelength properties of the spin $S = 3/2$ nearest-neighbor Heisenberg chain. We obtain an accurate value for the spin velocity $v = 3.87 \pm 0.02$, in agreement with experiment. Our results show conclusively that the model belongs to the same universality class as the $S = 1/2$ Heisenberg chain, with a conformal central charge $c = 1$ and critical exponent $\eta = 1$.   [S0031-9007(96)00504-2]

The study of one-dimensional spin-S Heisenberg Hamiltonians has received considerable attention in recent years. Their properties are important to experimentalists because they describe a number of materials with magnetic ions arranged in chains [1,2]. The first quasi-1D antiferromagnets with spin 3/2 which found experimental interest are $CsVCl_3$ [3] and $AgCrP_2S_6$ [4]. For theorists the spin models are among the simplest Hamiltonians where quantum fluctuations are crucial. However, only the special case $S = 1/2$ can be solved exactly [5]. In this case Luther and Peschel [6] found that the spectrum is gapless, there is no magnetic ordering in the ground state, and the spin correlation function $\omega(l) = \langle S_{i+l}^z S_i^z \rangle$ decays according to a power law $|\omega(l)| \sim 1/l^\eta$ with $\eta = 1$. Later Haldane [7] proposed that for half-odd-integer spin the Heisenberg Hamiltonian would behave as in the $S = 1/2$ case, i.e., no energy gap and power-law decay of the spin correlation function, while in the integer case the spectrum would have an energy gap and the spin correlations would decay exponentially. Early numerical work confirmed this conjecture [1,8,9] and power-law decay of the spin correlation was found for half-odd-integer spin, yet the exponent η seemed to be S dependent. When the powerful tools of conformal invariance started to be applied to one-dimensional quantum systems it became clear that the integrable $S = 1/2$ Hamiltonian at low energies is equivalent to the SU(2) symmetric Wess-Zumino-Witten (WZW) model with topological coupling constant $k = 1$ [10]. In this model, k is related to the central charge c by $c = 3k/(2 + k)$ and the critical exponent η is given by $3/(2 + k)$. It was also found [10] that a new class of integrable antiferromagnetic Hamiltonians with arbitrary spin [11] were equivalent to the WZW model with $k = 2S$.

Based on the SU(2) symmetry of the nonintegrable half-odd-integer spin Hamiltonians Schulz [12] suggested the following possible scenarios: (a) The half-odd-integer spin-S Heisenberg Hamiltonian belongs to the same universality class as the spin-S integrable model. In this case both models would have $c = 3k/(2 + k)$ and $\eta =$ $3/(2 + k)$ and $k = 2S$. This scenario was favored initially by Affleck [13]. (b) The spin-S integrable models represent unstable multicritical points in the phase diagram and the stable critical point is defined by the $S = 1/2$ Hamiltonian. Thus, the half-odd-integer spin-S Heisenberg model is expected to be equivalent to the $k = 1$ WZW model having $c = 1$ and $\eta = 1$, independent of the value of S. This position was favored by Schulz and later on by Haldane and Affleck [14,15].

Since the derivations of scenarios (a) and (b) involve several assumptions and approximations, unbiased numerical studies are needed to decide which one is correct. The $S = 3/2$ Heisenberg Hamiltonian is the simplest of the higher half-odd-integer spin models. Since there are 4 degrees of freedom per site, the longest chains that can be exactly diagonalized with present computer capabilities have 14 sites. Previous numerical studies conducted in such small chains gave conflicting results [16–18]. Moreo, [16] analyzing the behavior of spin correlation functions in lattices with $N \leq 12$, found $\eta \approx 0.6$, while Ziman and Schulz [17] obtained $\eta \approx 1$ by studying the behavior of the lowest triplet and singlet state energy gaps also in chains with $N \leq 12$. A Monte Carlo calculation of the spin correlation function [19] in chains with up to 128 sites provided exponents in disagreement with the SU(2) WZW scaling theory. The analysis of small systems is hampered by the presence of logarithmic corrections which modify the power-law dependence of various quantities in a significant way. In this Letter we will elucidate this problem numerically by studying sufficiently large systems that cannot be solved with exact diagonalization, and by Monte Carlo techniques only with considerable statistical error.

For this purpose we will use the density-matrix renormalization-group technique (DMRG) [20] keeping up to $m = 1200$ states per block and considering chains up to $N = 60$ sites. The large number of states m used in these calculations was dictated by (i) the use of periodic (instead of open) boundary conditions which requires more states [20] and (ii) the subsequent finite size analysis

of the data which involves power laws combined with logarithmic dependencies and thus requires high accuracy of the data even for the largest systems considered. For the largest chains we estimate that the ground state energy has an absolute error of less than 7×10^{-6}, by considering different m values. Our results for small systems, $N \leq 14$, agree with exact calculations [9,21,22] and the ground state energy is exact up to $N = 12$.

To calculate the conformal central charge c (or equivalently k) we account for the finite-size corrections of the ground-state energy per site, E_0/N, as derived from the WZW theory [15]

$$\frac{E_0}{N} = e_\infty - \frac{v\pi}{6N^2}\left[\frac{3k}{2+k} + \frac{3k^2}{8\ln^3(BN)}\right] - \frac{S}{N^4}. \quad (1)$$

The coefficient B depends on the effective coupling constant (see below) and can be dropped only in the large-N limit [23]. The last higher-order term reflects a finite size correction to the conformal charge. In principle Eq. (1) may be fitted with five free parameters; however, we found that more accurate results are obtained by an independent calculation of the spin velocity v and of B.

The spin velocity can be determined numerically from the excitation energy $\Delta_q = E(2\pi/N) - E(0) = v\sin(2\pi/N)$, where $E(2\pi/N)$ is the energy of the first excited state with the lowest nonzero momentum obtained from the spin excitation spectrum [24] and the Davidson algorithm [25] (with estimated absolute error $\simeq 10^{-2}$). Studying the behavior of Δ_q/N vs $\sin(2\pi/N)/N$, as shown in Fig. 1, to minimize the errors, we obtain a rather precise value for the spin velocity $v = 3.87 \pm 0.02$. This implies an enhancement factor of 1.29 with respect to the spin-wave result $v_{sw} = 2S = 3$. This factor is significantly lower than the value $\pi/2$ for the spin-1/2 chain (where $v_{sw} = 1$) thus implying that the quantum renormalization of the low-lying spin excitations is weaker.
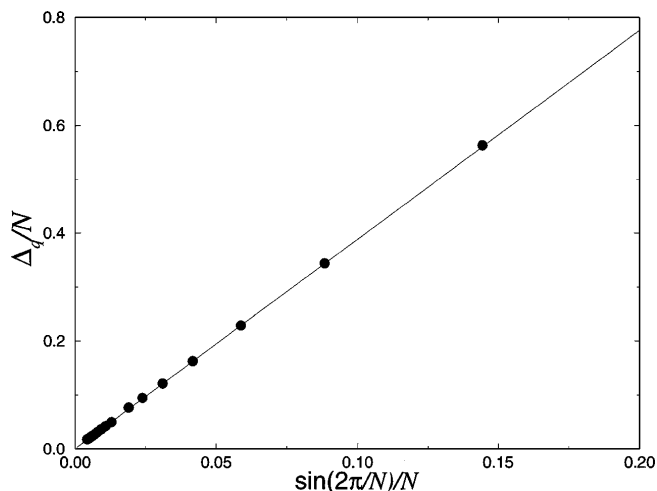

FIG. 1. Excitation energy Δ_q/N vs $\sin(2\pi/N)/N$. The linear interpolation yields the spin velocity (slope) $v = 3.87 \pm 0.02$ (full line).

Our v is higher than the value $v = 3.64 \pm 0.08$ given by Yamamoto [26]. The latter was calculated using a world-line Monte Carlo approach with larger error bars in the excitation energies ($\sim 10\%$ as estimated from the figures). The velocity is in good agreement with the measured spin-wave velocity $v = 1.26 v_{sw}$ for the spin-3/2 chain system $CsVCl_3$ [3]. Mutka, Payen, and Molinié [4] argued that their experimental results for the uniform susceptibility of the spin-3/2 chain system $AgCrP_2S_6$ are consistent with spin-1/2, i.e., supporting universality. Their value for the spin velocity $v = 1.53 v_s w$ appears too high in view of our results. The discrepancy between the experimental values may be partly attributed to the difficulty in extracting the exchange constant J from the uniform susceptibility [27].

The value of the coupling constant g of the conformal field theory can be determined directly by writing Eq. (1) in its equivalent form

$$\frac{E_0}{N} = e_\infty - \frac{v\pi}{6N^2}\left[\frac{3k}{2+k} + \frac{(2\pi g)^3}{\sqrt{3}\,k}\right] - \frac{S}{N^4}, \quad (2)$$

where

$$g(g_0, N, k) = \frac{g_0}{1 + \frac{4\pi g_0}{\sqrt{3}\,k}\ln(\frac{N}{l_0})} \quad (3)$$

and

$$B = \frac{e^{g_{\text{eff}}^{-1}}}{l_0}, \qquad g_{\text{eff}} = \frac{4\pi}{\sqrt{3}\,k}g_0. \quad (4)$$

From Eqs. (2) and (3) and the velocity given above we find $e_\infty = -2.82833(1)$, $k = 1.00(1)$, and the coupling constant $g_0 = g(l_0 = 20) = 0.055(5)$. The error was estimated using different subsets of the data. The constant S depends on the smallest system included in the fit, e.g., for $N \geq 12$ we found $S = 20$. From Eq. (4), $B = 0.6$ and $g_{\text{eff}} = 0.4$.

Using the previous values of v and B and from a three parameter fit of Eq. (1) using $N \geq 8$ we obtain consistently $e_\infty = -2.828\,33$, $k = 1 \pm 0.01$, and $S = 15$ (Fig. 2). Our ground-state energy is considerably lower than the energy $e_\infty = -2.8248$ obtained in a recent Monte Carlo study Ref. [28], where a $1/N^2$ scaling of the energy was assumed. From our results for k we conclude that $c = 1.00 \pm 0.01$.

To obtain the critical exponent we calculated the spin correlation function keeping 1000 states per block. The absolute error for the largest system is lower than 10^{-3}. We found that the scaling behavior obeyed by the spin 1/2 chain [23,29] is absent in this case and we extrapolated the finite-size data with a quadratic polynomial in $1/N^2$. The correlation function in the thermodynamic limit is shown in Fig. 3. We interpolated this correlation function using the theoretical prediction [15]

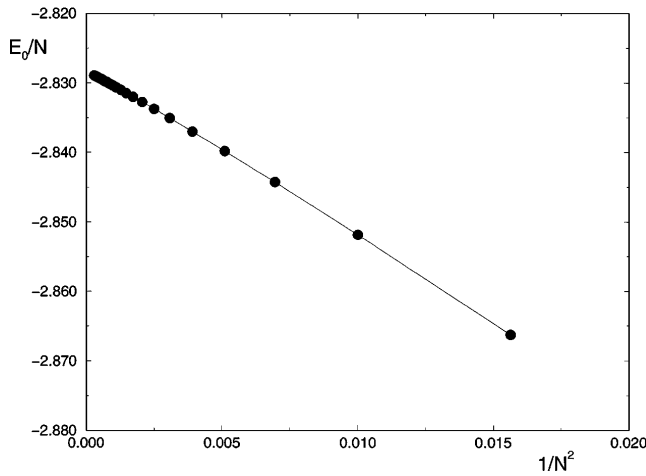$$\omega(l, \infty) = a\frac{\sqrt{\ln(Bl)}}{l^\eta}, \quad (5)$$

FIG. 2. Scaling of the ground state energy E_0/N. Interpolation including logarithmic corrections yields the central charge $c = 1.00 \pm 0.01$ and an extrapolated value $e_\infty = -2.828\,33$ (full line).

and obtained $a = 2.06$, $B = 0.56$, and $\eta = 1.02$. This fit is presented in Fig. 3 where we added the correlations for $S = 1/2$ to show that in both cases they have the same multiplicative logarithmic corrections, the coupling constant being smaller for $S = 1/2$ [23]. We note that $a = \omega(l_0, \infty)\sqrt{g_{\text{eff}}}\, l_0$ and B follows from Eq. (4). Using the value for g_{eff} given above and the extrapolated value for $\omega(l_0, \infty)$ we obtain $a = 2.07$ and $B = 0.6$. Thus the parameters obtained from the correlation function are in complete agreement, whithin error bars, with those obtained from the scaling of the ground-state energy.

On the other hand, if we assume $\eta = 1$, we can analyze $l\omega(l, \infty)/l_0\omega(l_0, \infty) = \sqrt{g(l_0)/g(l)}$. This ratio directly
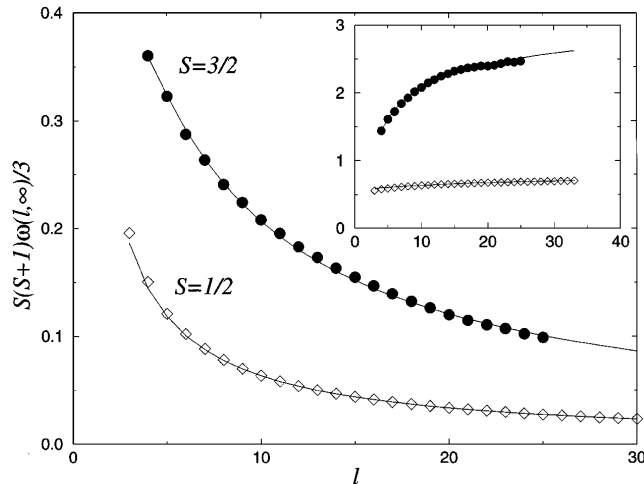

FIG. 3. Extrapolated and normalized spin correlation functions. The fit which includes the multiplicative logarithmic correction gives $\eta = 1.02$ (full line) and coefficients that are in agreement with those obtained from the scaling of the energy. The correlation function and fit of the spin-1/2 chain [23] is shown for comparison. Inset: normalized correlation functions multiplied by l, showing the logarithmic correction.

reflects the dependence on the coupling function [23] and a single parameter fit yields $g(l_0 = 20) = 0.052$.

The critical exponent η can also be calculated from the scaling of singlet and triplet excitation energies [15]:

$$\Delta_i = \frac{E_i - E_0}{N}$$

$$= \frac{2\pi v}{N^2}\left[\frac{\eta_i}{2} - \frac{\mathbf{S_L} \cdot \mathbf{S_R}}{\ln(BN)}\right] + \frac{b_i}{N^2 \ln^2(BN)}. \quad (6)$$

Here $\eta_i/2$ $(i = s, t)$ is the scaling dimension of the corresponding primary field, and $\mathbf{S_L}$ and $\mathbf{S_R}$ are the spin operators related to the energy levels of the conformal field theory describing the fixed point, with spin quantum numbers s_L and s_R. According to the WZW mapping

$$\mathbf{S_L} \cdot \mathbf{S_R} = \frac{1}{2}\left[s(s + 1) - s_L(s_L + 1) - s_R(s_R + 1)\right], \quad (7)$$

where s is the total spin number. The triplet state $s = 1$ and the first singlet excitation $s = 0$ (for both cases $s_L = s_R = 1/2$) become degenerate in the thermodynamic limit. Therefore, if we take the appropriate linear combination of Eq. (6) for these excitations, the leading logarithmic corrections are canceled out:

$$\Delta = \frac{1}{4N}\left[(E_s - E_0) + 3(E_t - E_0)\right]$$

$$= \frac{\pi v \eta}{N^2} + \frac{b}{N^2 \ln^2(BN)}. \quad (8)$$

This quantity has been used before in Ref. [17] to estimate η using three system sizes, i.e., $N = 8$, 10, and 12 sites with the result $\eta \simeq 1$. We reached an excellent interpolation of our data (including a S'/N^4 term), shown in Fig. 4, leading to $\eta = 1.018$, $b = b_s - 3b_t = -5.4$, and $S' = 80$.
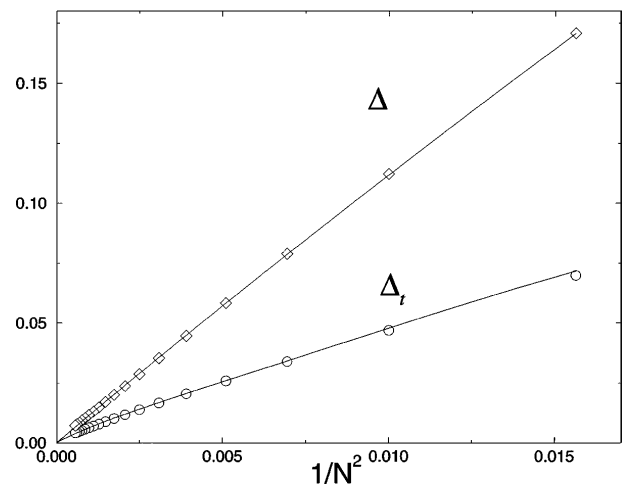

FIG. 4. Scaling of the triplet gap (circles) and the combined gap Δ (diamonds). Equations (6) and (8) were used to extract the exponent η (full lines).

We also obtained a good fit for the triplet finite-size gap (Δ_t), also shown in Fig. 4, but we were forced to add the subleading terms $\left(\sim[\ln\ln(BN)]^2/\ln^4(BN)\right.$ and $\left.S''/N^4\right)$ to obtain convergence. In this case our results are $\eta = 0.977$, $b_t = 34$, and $S'' = 83$. For the interpolation we have used the values for the velocity and B calculated earlier.

In conclusion, we have found very accurate values for the spin velocity, the central charge c, and the critical exponent η for the Heisenberg Hamiltonian with $S = 3/2$ using the DMRG technique that allowed us to study sufficiently large chains with negligible error. We found $c = 1.00 \pm 0.01$ and $\eta = 1.02 \pm 0.02$ which shows, within error bars, that this model belongs to the same universality class as the $S = 1/2$ Heisenberg model and the WZW model with $k = 1$. The $k = 2S = 3$ WZW model with $c = 9/5$ and $\eta = 3/5$ can be ruled out. These values have been obtained by an analysis of the ground-state energy, the lowest singlet and triplet excitation energies, as well as the spin correlation function. We have found an excellent agreement between the parameters deduced from these different data sets. Apart from a larger coupling constant the correlation function of the spin-3/2 chain has the same multiplicative logarithmic corrections as for spin $1/2$.

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