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**LETTER TO THE EDITOR**

# Finite size study of the spin-$\frac{1}{2}$ dimerised Heisenberg chain

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**Abstract.** We present the results of a finite size analysis of the one-dimensional spin-$\frac{1}{2}$ dimerised Heisenberg chain. The value of the gap exponent, $\nu$, is obtained using two extrapolation procedures. When logarithmic corrections are taken into account, we obtain the values $\nu = 0.668 \pm 0.001$ and $\nu = 0.667 \pm 0.002$, in good agreement with the conjectured value $\nu = \frac{2}{3}$. We compare these results with those obtained assuming a pure power-law behaviour.

In this letter, we are concerned with the estimation of the exponent, $\nu$, which characterises the opening of the gap in the excitation spectrum of the one-dimensional (1D) dimerised spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chain at zero temperature. The Hamiltonian is

$$H = J \sum_{i=1}^{N} \{1 + (-1)^i \delta\}\{\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \tfrac{1}{4}\} \tag{1}$$

where the alternation parameter, $\delta$, is restricted to $|\delta| \leqslant 1$ and where $\boldsymbol{S}_i$ is the spin-$\frac{1}{2}$ vector operator at site $i$. The exchange coupling is antiferromagnetic and the sum runs over the $N$ sites of the chain, which we shall assume even.

Cross and Fisher (1979) have predicted a power-law behaviour for the gap, $\Delta$, in the excitation spectrum of (1). Near criticality ($\delta \to 0$), $\Delta \sim |\delta|^{\nu}$ with $\nu = \frac{2}{3}$. The 1D Hamiltonian (1) has been shown by Kohmoto *et al* (1981) to be equivalent to the 2D Ashkin-Teller model which, at the bifurcation point (Kadanoff 1980), corresponds to the 2D four-state Potts model for which marginality effects are important. These effects are associated either with the presence of a dilution field (Nauenberg and Scalapino 1980) or with umklapp scattering (Black and Emery 1981). As a consequence of these marginality effects, logarithmic correction terms to the above power-law behaviour are expected. These corrections have been invoked (Hamer 1981) to explain the discrepancy between the estimated values of $\nu$ and the value, which den Nijs (1979) has conjectured, of $\frac{2}{3}$. The reader is referred to the paper of Hu (1980) for a list of references concerning the estimation of this exponent. We add to this list the result of Fields (1979; $\nu = 0.86$), the result of Hamer (1981; $1/\nu = 1.40 \pm 0.03$), the estimation of Herrmann (1981; $1/\nu = 1.48 \pm 0.01$) and the recent calculations of Alcaraz and de Felício (1984; $1/\nu = 1.42 \pm 0.05$). In this letter, we present an analysis of finite size data which takes into account logarithmic corrections to scaling in the form suggested by the work of Blöte and Nightingale (1982). We estimate the values of $\nu$ and $1/\nu$

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using the Vanden Broeck and Schwartz (1979) approximants (VBS) and $1/N^x$ fit. We also compare the results with those obtained assuming a pure power-law behaviour.

In order to introduce the main aspects of our calculations, we first write the Hamiltonian (1) in terms of spinless fermion variables. Using the Wigner-Jordan transformation, one obtains (Soos 1965):

$$H = -J\sum_{i=1}^{N} n_i + J\sum_{i=1}^{N}\{1+(-1)^i\delta\}n_i n_{i+1} + \frac{J}{2}\sum_{i=1}^{N-1}\{1+(-1)^i\delta\}\{f_i^\dagger f_{i+1} + \text{CC}\}$$

$$-\frac{J}{2}(-1)^\sigma\{1+\delta\}\{f_1^\dagger f_N + \text{CC}\}. \tag{2}$$

The spinless fermion operator $f_i^\dagger$ ($f_i$) creates (annihilates) a particle at site $i$ and $n_i = f_i^\dagger f_i$; $\sigma = \sum n_i$ is the operator for the total number of particles. The sign of the last term in (2) thus depends on the parity, $\alpha$, of the total number of particles. The Hamiltonian (2) can also be written in $k$ space. The set of allowed values of $k$ is obtained from the periodic boundary conditions (PBC) imposed on the original spin Hamiltonian (1) (i.e. $\boldsymbol{S}_{N+1} = \boldsymbol{S}_1$). This yields

$$\exp(ikN) = -(-1)^\alpha. \tag{3}$$

The boundary conditions imposed on the spinless fermion system thus depend upon the parity of $\alpha$; that is, PBC for odd values of $\alpha$ ($f_{N+1} = f_1$) and antiperiodic boundary conditions (APBC) for even $\alpha$ ($f_{N+1} = -f_1$). According to (3), states with different numbers of particles, for instance $m$ and $m+1$ particles, do not share the same set of $k$'s. In the half-filled band case, neither do two consecutive cell sizes, $N$ and $N+2$, share the same set. This may affect the extrapolation of finite cell results, such as those for the ground-state energy and for the gap in the excitation spectrum, to the $N \to \infty$ limit. The situation may be improved by using modified boundary conditions (MBC) (Jullien and Martin 1982). This procedure has been shown to be powerful in reproducing some exact results such as the essential singularity exponent, $s = \frac{1}{2}$, that characterises the opening of the gap in the excitation spectrum of the 1D Heisenberg-Ising model (Spronken *et al* 1981) and the essential singularity exponent, $s = 1$, of the 1D Hubbard model (Uzelac 1984, Fourcade and Spronken 1984). When MBC are used the $k$'s are shifted so that the set of allowed $k$'s is, for a given $N$, independent of the number of particles, and such that cells of different size share at least one $|k|$, which we shall take as $|k| = \pi/2$. It is easily seen that this is achieved provided the quantities $-(-1)^\sigma$ and $-(-1)^\alpha$, in (2) and (3), are replaced by $(-1)^{N/2}$. Note that the MBC, when applied to the 1D dimerised $XY$ chain, yields, for the gap: $\Delta_N(\delta) = 2|\delta|$; the exact result as $N \to \infty$ (Fields 1979) is then exactly recovered for all cell sizes.

We have applied the MBC to the spinless fermion Hamiltonian (2). The ground-state energies, for $N/2$ and $N/2+1$ particles, are obtained using the Lanczös algorithm (Whitehead *et al* 1977). An important aspect of this method is that the ground-state energy, $E$, converges rapidly as one increases the number of Lanczös steps. There is, in addition, another important result: the average values of some operators (Fourcade and Spronken 1984) also converge rapidly. This is the case of the operator ($J = 1$)

$$D = \sum_{i=1}^{N}(-1)^i n_i n_{i+1} + \frac{1}{2}\sum_{i=1}^{N-1}(-1)^i\{f_i^\dagger f_{i+1} + \text{CC}\} + \frac{1}{2}(-1)^{N/2}\{f_1^\dagger f_N + \text{CC}\} \tag{4}$$

which, according to a theorem due to Feynman (1939), is the derivative of the ground-state energy with respect to the alternation parameter $\delta$. Typical accuracy for the

ground-state energy and its derivative is of the order of nine significant figures. As a consequence, the gap, defined as ($J = 1$):

$$\Delta_N(\delta) = 2\{E(\delta, \tfrac{1}{2}N+1) - E(\delta, \tfrac{1}{2}N)\} \tag{5}$$

and its derivative, $\Delta'_N(\delta) = \partial\Delta_N(\delta)/\partial\delta$ can be computed with great accuracy. In (5), $E(\delta, m)$ stands for the ground-state energy of a chain filled with $m$ particles and we have made used of the electron-hole symmetry property of the spectrum of $H$.

In figure 1 we compare the results obtained for the inverse of the gap, $\Delta_N^{-1}(0)$, using the MBC (case A) and the usual boundary conditions (case B). This quantity apparently approaches a straight line, $\Delta_N^{-1}(0) = a + bN$, for all $N$'s in the case A and for $N \geqslant 8$ in the case B. To conclude that the MBC results simulate the asymptotic limit ($\Delta_N^{-1}(0) \sim N$) can be misleading, however. Additional size dependences of the results are expected the case B. To conclude that the MBC results simulate the asymptotic limit ($\Delta_N^{-1}(0) \sim N$) $\Delta_N^{-1}(0) \sim N + O(N/\ln N)$. Similar effects could also occur in case A.

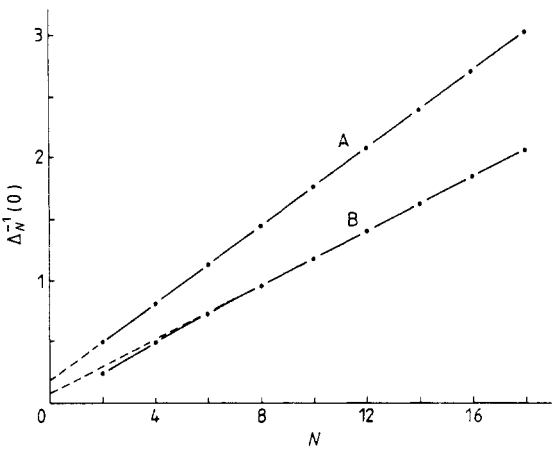


**Figure 1.** Plot of the inverse of the gap, $\Delta_N^{-1}(0)$, as a function of the size $N$: A, the MBC results; B, the PBC results.

For the range studied here ($2 \leqslant N \leqslant 18$), the apparent linear behaviour of the MBC results suggests that the quantity $Q_N^{-1}(\delta) = \Delta_N^{-1}(\delta) - a$ satisfies a modified phenomenological renormalisation group equation, $NQ_N(\delta) = MQ_M(\delta')$ (Nightingale 1982). Indeed, we find that the quantity $NQ_N(\delta)$, when plotted as a function of $\delta$, yields a set of curves all intersecting at $\delta = 0$, the expected critical value of the alternation parameter. Note that a similar plot of $N\Delta_N(\delta)$ yields a set of curves intersecting at negative values of $\delta$, a result which violates the symmetry property of the spectrum of the Hamiltonian upon the exchange $\delta \leftrightarrow -\delta$. Obviously, the quantities $Q_N^{-1}(0)$ and $\Delta_N^{-1}(0)$ become identical as $N \to \infty$. Accordingly, the above results suggest that a finite size study, at $\delta = 0$, of the quantity $Q_N^{-1}(\delta)$ should yield information about the infinite system gap exponent, $\nu$. We write the finite size scaling equation for the quantity $Q_N^{-1}(\delta)$ as

$$Q_N^{-1}(\delta) = NF(\delta Z) \tag{6}$$

where $F(Z\delta)$ is a universal scaling function which can depend on the boundary

conditions (Privman and Fisher 1984). At $\delta = 0$, one has $F(0) = b$. The quantity $Z$, in equation (6), is $Z = N^{1/\nu}$ for the pure power-law case (Fisher and Barber 1972) and $Z = [N/(\ln N)^{1/2}]^{1/\nu}$ when logarithmic corrections are taken into account. In this last case, we have neglected, in (6), all additional corrections to scaling in order to keep the expression as simple as possible (Blöte and Nightingale 1982, Herrmann 1981). The calculation of $Q_N^{-1}(\delta)$ is affected by unavoidable lack of accuracy in determining the quantity $a$. This can be avoided by differentiating (6). One obtains, at $\delta = 0^+$:

$$Q'_N(0^+)/Q_N^2(0^+) = \Delta'_N(0^+)/\Delta_N^2(0^+) \sim ZN \tag{7}$$

where $Z$ is defined above and $\Delta_N(0^+)$ and $\Delta'_N(0^+)$ are computed from (4) and (5). The gap exponent, $\nu$, is obtained from a two-point fit ($4 \leqslant N \leqslant 18$) and the resulting sequence of values for the exponent is extrapolated to the $N \to \infty$ limit. In table 1, we give the results obtained using the VBS approximants to $\nu$. The same procedure was also applied to estimate $1/\nu$. In table 2 we give the results and compare them with those obtained using another extrapolation procedure (fit of the sequence with $C_1 + C_2/N^x$). We also give an estimation of the errors.

The results can be summarised as follows. (1) The values obtained assuming a pure power law are in agreement with those previously obtained by other authors;

**Table 1.** The VBS approximants to $\nu$ when (A) a pure power-law behaviour is assumed and when (B) logarithmic corrections are taken into account. The left-hand columns list the values of the exponent, $\nu_{N,N+2}$, obtained from a two point fit for $N = 4, 6, \ldots, 16$.

| | | | | |
|---|---|---|---|---|
| | 1.106 021 | | | |
| | 0.982 029 | 0.873 762 | | |
| | 0.924 231 | 0.842 037 | 0.732 605 | |
| A | 0.890 295 | 0.823 107 | 0.723 840 | 0.707 328 |
| | 0.867 748 | 0.810 250 | 0.718 113 | |
| | 0.851 552 | 0.800 819 | | |
| | 0.839 275 | | | |
| | | | | |
| | 0.756 096 | | | |
| | 0.727 885 | 0.696 968 | | |
| | 0.713 134 | 0.690 750 | 0.667 847 | |
| B | 0.704 243 | 0.686 737 | 0.668 602 | 0.668 380 |
| | 0.698 346 | 0.683 970 | 0.668 286 | |
| | 0.694 165 | 0.681 950 | | |
| | 0.691 050 | | | |

**Table 2.** Summary of the results obtained using the VBS approximants and the fit with $C_1 + C_2/N^x$ in the case of (A) a pure power-law behaviour and when (B) logarithmic corrections are taken into account.

| | A | | B | |
|---|---|---|---|---|
| | VBS | $C_1 + C_2/N^x$ | VBS | $C_1 + C_2/N^x$ |
| $1/\nu$ | $1.42 \pm 0.02$ | $1.3675 \pm 0.0002$ | $1.497 \pm 0.002$ | $1.507 \pm 0.003$ |
| $\nu$ | $0.71 \pm 0.01$ | $0.768 \pm 0.002$ | $0.668 \pm 0.001$ | $0.667 \pm 0.002$ |

note, however, that the estimated values of $\nu$ and $1/\nu$ depend significantly on the extrapolation procedures used. (2) When logarithmic corrections are taken into account, both extrapolation procedures yield essentially the same results which are in excellent agreement with the conjectured value of $\nu$, the difference being less than 0.2%. The difficulties in computing the eigenvalues of the Hamiltonian increase rapidly with the size of the cell and $N = 18$ is about the largest size which it has been possible to compute up to the present time. Accordingly, it is almost impossible to prove the presence of logarithmic terms, and the results shown in table 2 (case B) are indeed not final: they cannot be used to definitively show the validity of the den Nijs conjecture. However, they clearly support it.

We have also evaluated the exponent $\nu$ using the Callan-Symansik expression (Hamer and Barber 1981) and the derivative of the gap. The results obtained, which are similar to those shown in table 2, will be published elsewhere along with an extensive study of the ID dimerised Heisenberg chain for arbitrary values of the alternation parameter $\delta$.

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