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1991 J. Phys.: Condens. Matter 3 3343

(http://iopscience.iop.org/0953-8984/3/19/013)

J. Phys.: Condens. Matter 3 (1991) 3343–3352. Printed in the UK

Critical behaviour of coupled spin chains

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Received 13 November 1990, in final form 12 February 1991

Abstract. We investigate, using numerical computation of the eigenvalues of short chains, the critical behaviour of two composite spin models, which interpolate smoothly between isotropic Heisenberg chains with different values of S. For the first model which interpolates between $S = \frac{1}{2}$ and $S = \frac{3}{2}$ we find that the model is critical over the whole range and the values of the central charge and critical exponents (scaling dimensions) appear to be constant in the thermodynamic limit. In the second model, which interpolates between $S = \frac{1}{2}$ and $S = 1$ we find that, except at $S = \frac{1}{2}$, the central charge is effectively zero, implying a non-critical behaviour.

1. Introduction

Over the last few years critical properties of spin models have been studied with increasing interest. There are a number of reasons for this interest, and one of them is the conjecture made by Haldane [1] some while ago of the difference between integer spin and half-integer spin antiferromagnets. Another reason for this interest is the recent discovery of the conformal invariance [2] at the transition point of the models exhibiting a second order phase transition. Spin models provide a good testing ground for studying the consequences [3] of this invariance.

A field of research which quite recently has become a part of the studies concerning criticality is that of integrable models [4]. An effective use [5] of the methods based on Bethe's ansatz has proved to be a powerful way of evaluating quantities characteristic of conformally invariant models. The usefulness of these methods relies on the fact that the spectrum of the integrable SU(2) spin-S models consists [6] of a gapless doublet of $S = \frac{1}{2}$ spin waves which form the (two-particle) singlet and triplet excitations of physical states.

The critical exponents of the integrable spin models [7] are smooth functions of the length of the spin S. In contrast with this, the isotropic and nearly isotropic Heisenberg antiferromagnets with a half-integer spin are all believed [1, 8] to have the same critical exponents, and those with an integer spin are believed [1, 8] to be non-critical. A slightly worrying feature of the original [8] analysis leading to this result is, however, that when applied to the integrable spin models it produces [9] for these the same results as for the Heisenberg antiferromagnets, i.e. half-integer spin models should be critical but integer spin models non-critical. The analysis was based on a mapping of the models to a quantum field theory model, the nonlinear σ model.

0953-8984/91/193343+10$03.50

Subsequently a modified [10] form of the method has been developed which gives more insight into this very subtle problem. Based on the modified version of the analysis [10], and also on other even earlier arguments [11], it is now expected that the integrable spin models correspond to multicritical points in the space of couplings. Any perturbation of the couplings specific to the integrable models will drive the models away from the integrable points, and the spectra and the correlation functions of the models will change accordingly. In a model with an integer spin these perturbations will cause a gap to appear in the excitation spectrum and the correlation functions will decay exponentially. In a model with a half-integer spin the spectrum will remain gapless, i.e. it is critical, and the critical exponents of the correlation functions will change to become those of the $S = \frac{1}{2}$ isotropic Heisenberg antiferromagnet.

There is now also numerical evidence [11–13] for the different critical behaviour of the integrable and non-integrable spin models. The work of Ziman and Schulz [11] in particular is very interesting, because they have found a method of getting rid of the leading finite size correction, which is logarithmic, to the scaling dimensions of the relevant operators. The idea of Ziman and Schulz is to consider a suitable linear combination of the primary singlet–triplet gap and the smallest singlet–singlet gap, and is based on the degeneracy in the infinite length limit of these gaps. In this way they were able to show in a model which interpolates between the integrable $S = \frac{3}{2}$ model and the usual $S = \frac{3}{2}$ Heisenberg model that whenever the model is away from the integrable point its critical exponents are those of the $S = \frac{1}{2}$ Heisenberg model.

In the analysis of spin models with spin higher than a half the composite spin representation has been shown [9, 14, 15] to provide new insights. Having at each lattice site an equal number of shorter spins, the original spin problem is now replaced by that of a set of coupled chains with shorter spins. It is then possible to have at each site a whole sequence of total spins. The composite spin representation can however be used because the low lying states of the composite spin Hamiltonian are [9, 14] in the subspace of the largest total spin. The lowest part of the spectrum of a $S = 1$ model for example is exactly given by two coupled $S = \frac{1}{2}$ chains. A $S = \frac{3}{2}$ model can be represented by either three coupled $S = \frac{1}{2}$ chains or two coupled chains with $S = \frac{1}{2}$ and $S = 1$, respectively. Varying the couplings of the chains makes it possible to interpolate between models with different spin lengths. It is natural to extend the previous work [9, 14], and ask in a different way how the critical behaviour is changed when we interpolate between models with different spin lengths.

A convenient way to study the critical behaviour of spin models is to calculate [11–13] their conformal anomaly or central charge and the anomalous or scaling dimensions of the relevant operators. The central charge c, which is used to divide the models into different universality classes, can be easily determined from the finite size corrections to the ground state energy of the model. Conformal invariance predicts that, for a chain of N sites, the ground state energy per site, $E_0(N)N^{-1}$, approaches its asymptotic value ϵ_∞ as [2]

$$E_0(N)N^{-1} = \epsilon_\infty - \tfrac{1}{6}\pi c v N^{-2} + O(N^{-3}) \tag{1.1}$$

where v is the spin wave velocity.

The scaling dimensions of the relevant operators can be determined from the finite size corrections to the excitation energies. The excited states related to an operator ϕ form 'towers' characterized by the scaling dimension X_ϕ and the spin S_ϕ of that operator such that the excitation energies and the corresponding momenta can be written as [2]

$$E_{n,n'}(N) = E_0(N) + \frac{2\pi v}{N}(X_\phi + n + n') + \mathcal{O}(N^{-2})$$
$$P_{n,n'}(N) = \frac{2\pi}{N}(S_\phi + n - n') + \mathcal{O}(N^{-2}) \qquad n, n' = 0, 1, 2, \ldots \tag{1.2}$$

In the work reported in this paper we have only considered the lowest excited states with $n = n' = 0$, i.e. excitation energies

$$\epsilon \equiv E_{0,0}(N) - E_0(N) = \frac{2\pi v}{N} X_\phi + \mathcal{O}(N^{-2}). \tag{1.3}$$

In this paper we shall analyse the composite spin models by studying their possible conformal invariance. We wish to determine in particular the crossover from the $S = \frac{1}{2}$ behaviour of the decoupled chains to the $S = \frac{3}{2}$ behaviour of the 'completely' coupled chains. This crossover will be contrasted with that of the supposedly non-critical $S = 1$ chain composed of two coupled $S = \frac{1}{2}$ chains. In section 2 we shall introduce the composite spin models which are used in this work. The numerical results for the central charge and for the scaling dimensions will be given in section 3, and the results will be discussed in section 4.

2. Composite spin models

A general spin model with isotropic nearest neighbour couplings can be defined as

$$H = \sum_{i=1}^{N} \sum_{k=0}^{2S} a_k (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^k \tag{2.1}$$

where a_k are arbitrary constants and $|\boldsymbol{S}_i| = S$. The usual Heisenberg model corresponds to the case when only a_1 is different from zero. The integrable spin models correspond to particular choices of the constants a_k which are different for each S. In this work we shall concentrate on the Heisenberg case, but a similar analysis could be made [14] of the more general model.

As discussed in the previous section the composite spin models can also be viewed as coupled spin chain problems. The simplest case is that of two chains, one with spins $\boldsymbol{\sigma}_i$ the other with spins $\boldsymbol{\tau}_i$. The operators $\boldsymbol{\sigma}_i$ and $\boldsymbol{\tau}_i$ are not necessarily spin-$\frac{1}{2}$ operators, the only restriction we impose on these operators is that all spins on the same chain are equal, i.e. $|\boldsymbol{\sigma}_i| = \sigma$ and $|\boldsymbol{\tau}_i| = \tau$ independent of the site i. This ensures that at $\lambda = 0$ and $\lambda = 1$ the total spin at each site is a good quantum number. The Hamiltonian of the simplest non-trivial coupled two-chain problem can be expressed in the form

$$H = \sum_i \{\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1} + \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_{i+1} + \lambda \boldsymbol{\sigma}_i \cdot \boldsymbol{\tau}_{i+1} + \lambda \boldsymbol{\tau}_i \cdot \boldsymbol{\sigma}_{i+1}\}. \tag{2.2}$$

The coupling terms between the two chains are in (2.2) multiplied by the 'interpolation parameter' λ, and they will be treated as a perturbation of the uncoupled chains.

At $\lambda = 0$ the model (2.2) obviously describes two uncoupled chains. The properties of the model now depend on the spin lengths of the individual chains, σ and τ. We have shown earlier [9, 14] that if e.g. $\sigma = \tau = \frac{1}{2}$, the lowest part of the spectrum at $\lambda = 1$ is identical to that of a single spin-1 chain. It is expected in general that the two-chain model will be at $\lambda = 1$ a good representation of the single chain model with spin $S = \sigma + \tau$. If $\sigma = \tau = \frac{1}{2}$ we shall call the Hamiltonian (2.2) the $(2 \times \frac{1}{2})$ model.

Hamiltonian (2.2) can easily be generalized to include three chains with spins σ_i, τ_i and ρ_i. In this case the Hamiltonian is

$$H = \sum_i \{\rho_i \cdot \rho_{i+1} + \sigma_i \cdot \sigma_{i+1} + \tau_i \cdot \tau_{i+1} + \lambda\sigma_i \cdot (\tau_{i+1} + \rho_{i+1}) + \lambda\tau_i \cdot (\rho_{i+1} + \sigma_{i+1}) + \lambda\rho_i \cdot (\tau_{i+1} + \sigma_{i+1})\}. \tag{2.3}$$

Let us assume that (2.3) describes the $(3 \times \frac{1}{2})$ model with $\sigma = \tau = \rho = \frac{1}{2}$. At $\lambda = 0$ the chains are again decoupled. Clearly at $\lambda = 1$ the coupling will be so strong as to destroy the individuality of the chains. Varying λ between these two limiting values will cause the properties of the model to cross over from the spin-$\frac{1}{2}$ behaviour to the spin-$\frac{3}{2}$ behaviour.

At $\lambda = 0$ the finite size corrections to the ground state and excitation energies will appear independently in all three of the uncoupled chains. Therefore the central charge will be three times that of the $S = \frac{1}{2}$ Heisenberg chain, $c(\lambda = 0) = 3$. At $\lambda = 1$ the central charge should be equal to that of the $S = \frac{3}{2}$ Heisenberg chain, i.e. $c(\lambda = 1) = 1$ supposing that the critical properties of the two Heisenberg models are the same. We shall show in the next section our numerical result for $c(\lambda)$, $0 \leqslant \lambda \leqslant 1$.

The scaling dimension of both the $S = \frac{1}{2}$ and $S = \frac{3}{2}$ Heisenberg chain is $X = \frac{1}{2}$. Since in the decoupled three-chain problem the lowest excitations arise from exciting only one of the chains, the composite spin model (2.3) should have [19] $X(\lambda = 0) = X(\lambda = 1) = 0.5$. Unfortunately, there are logarithmic terms in the finite size dependence of the excitation energies which make the evaluation of X rather difficult. We shall follow Ziman and Schulz and consider, instead of the lowest singlet, Δ_s, and triplet, Δ_t, gaps separately, the linear combination

$$\Delta = \tfrac{1}{4}(\Delta_s + 3\Delta_t). \tag{2.4}$$

Since the singlet and triplet excitations are predicted to be degenerate in the thermodynamic limit, Δ defined by (2.4) should give the correct scaling dimension. The advantage of using (2.4) is that the leading logarithmic corrections are cancelled, and a much better estimate of the scaling dimension should be achieved.

3. Numerical results

We have solved numerically the few lowest eigenenergies of the models (2.2) and (2.3). In these calculations for finite chains we have imposed periodic boundary conditions and determined by exact diagonalization or by the Lanczos method the few lowest eigenstates in sectors characterized by the z-component of the total spin and by the momentum. For the $(2 \times \frac{1}{2})$ model (2.2), we have results for up to $N = 10$ sites, and for the $(3 \times \frac{1}{2})$ model (2.3), we have results for up to $N = 8$. At the points $\lambda = 0$ and $\lambda = 1$ which correspond to the $S = \frac{1}{2}$ and $S = 1$ $(\frac{3}{2})$ Heisenberg models, respectively, our results coincide with the published numerical data for these models which exist for up to $N = 18$ in the $S = \frac{1}{2}$ case [16], and for up to $N = 16$ (12) in the $S = 1$ ($\frac{3}{2}$) case [13]. In all cases the ground state of the system is a spin singlet state with zero momentum, and the first excited state is, at least in the range of λ we consider, in the triplet spin sector.

We shall first consider the $(3 \times \frac{1}{2})$ model (2.3). In order to find if this model is critical, we have calculated its ground state energy for N and $N+2$, and inferred from these the central charge c by using (1.1). In this way we get successive estimates for c. The numerical value of the central charge depends also on the spin wave velocity which we have determined by numerically calculating the finite size spectrum. To improve the accuracy we have assumed that for finite chains the spectrum can be expressed in the form

$$\begin{aligned} \epsilon(k) &= \Delta(\lambda, N)\frac{k}{\pi} + v(\lambda, N)\sin k \\ v(\lambda, N) &= v_0(N) + v_1(N)\lambda + v_2(N)\lambda^2 \end{aligned} \tag{3.1}$$

where $\Delta(\lambda, N)$ is the gap between the lowest $k = 0$ and $k = \pi$ states which is finite for all $N < \infty$. We have also assumed that $v(\lambda, N)$ has a well defined expansion in λ, and have found it is enough to include the terms up to the second order.

We have assumed that $v_j(N)$, $j = 0, 1, 2$, have well defined expansions in N^{-1}, and by using polynomial extrapolation to the limit $N \to \infty$ we find that

$$v(\lambda) \equiv v(\lambda, \infty) = \tfrac{1}{2}\pi + 2.1126\lambda + 0.2526\lambda^2 \tag{3.2}$$

for the $(3 \times \frac{1}{2})$ model.

We show the central charge in figure 1 as a function of the interpolation parameter λ. It appears from figure 1 that at $\lambda = 1$ the central charge approaches the value $c = 1$ which is the same as that of the $S = \frac{1}{2}$ Heisenberg model. This suggests that the $S = \frac{1}{2}$ and $S = \frac{3}{2}$ Heisenberg chains are in the same universality class, in agreement with [11]. We note in figure 1 that for a given N there is a range of λ over which c remains effectively constant at the $S = \frac{3}{2}$ value. This range increases as N increases and in the limit $N \to \infty$ seems to become the whole interval $0 < \lambda \leqslant 1$. This result supports our previous findings [9, 14] for the composite spin model. At $\lambda = 0$ the central charge approaches the expected value $c = 3$. To investigate better the scaling of c as a function of N we show in figure 2 a plot of c as a function of $(\ln N)^{-3}$ which is the leading correction to c in $S = \frac{1}{2}$ type models. We show in figure 2 only one intermediate value of λ, $\lambda = 0.25$, because for $\lambda > 0.25$ the curves approach the $\lambda = 1$ curve vary rapidly and would appear as one curve. This figure shows clearly the two limits in the scaling, $c(\lambda = 0) = 3$ and $c(\lambda > 0) = 1$.

The other quantity we have determined for the $(3 \times \frac{1}{2})$ model is the scaling dimension of the operator responsible for the primary gap in the finite size excitation spectrum. Because of the large finite size corrections in the primary gap which make the evaluation of the scaling dimension very difficult [11, 12] we have used the method of [11] as explained in the introduction.

We show in figure 3 the scaling dimension related to the singlet–triplet and singlet–singlet gaps, and also the result of taking the linear combination of the two. We show the results for only $N = 4$ and $N = 8$ because the singlet–triplet curve for $N = 6$ would be too close to the $N = 8$ curve to be clearly seen. It is evident that drawing on the

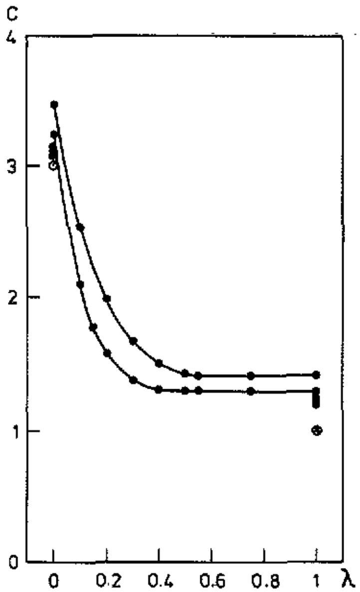

Figure 1. Central charge of the $(3 \times \frac{1}{2})$ model. Filled circles mark the values which are determined from calculated values for N and $N+2$. The upper curve is the result for $N = 4$, and the lower curve for $N = 64$. For $\lambda = 0$ and $\lambda = 1$ there are results for $N = 8$ and $N = 10$, and the expected limiting values are also marked.

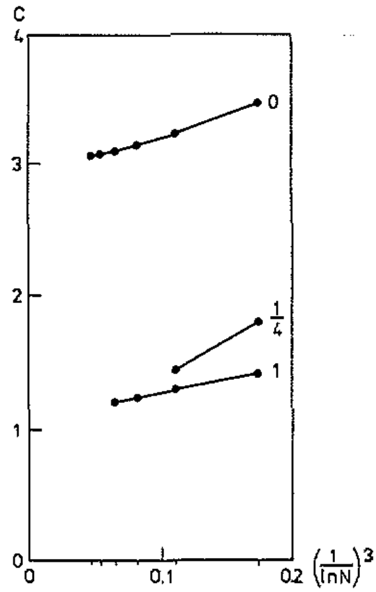

Figure 2. Scaling against $(\ln N)^{-3}$ of the extrapolated central charge of the $(3 \times \frac{1}{2})$ model. The numbers on the right refer to the values of λ.

singlet–triplet results only [12] would lead to an erroneous extrapolation of the scaling dimension, convergence is so slow that extremely long chains would be needed in order to find the true asymptotic behaviour. In contrast with this, the linear combination of the two scaling dimensions seems to converge very rapidly, giving reliable estimates already for rather short chains. This result is, of course, very much in agreement with the findings of Ziman and Schulz [11], who, however, had a different model and used a completely different numerical procedure. Our numerical results, which for general λ exist only for N up to 8, are consistent with a scaling dimension $X = 0.5$ for all $0 \leqslant \lambda \leqslant 1$ in the $N \to \infty$ limit. This is another indication of the $S = \frac{1}{2}$ like critical behaviour being generic for half-integer spin systems.

According to [11] the leading correction to the scaling dimension should be proportional to $(\ln N)^{-2}$. We have therefore plotted in figure 4 the scaling dimension as a function of $(\ln N)^{-2}$. We show the results mainly for $\lambda = 0$ and $\lambda = 1$, the curves for other values of λ lie between the $\lambda = 0$ and $\lambda = 1$ curves. For the available chain lengths the scaling dimensions of the singlet–triplet and singlet–singlet gaps are very far from their assumed asymptotic values. The linear combination of the two seems to scale quite well even for the short chains we could do numerically, the $\lambda = 0$ curve is almost flat, but it is so close to the asymptotic value that the question of scaling is not very relevant.

Our results for the $(3 \times \frac{1}{2})$ model which interpolates between the $S = \frac{1}{2}$ and $S = \frac{3}{2}$ Heisenberg chains seem strongly to indicate that this model is critical for all $0 \leqslant \lambda \leqslant 1$.

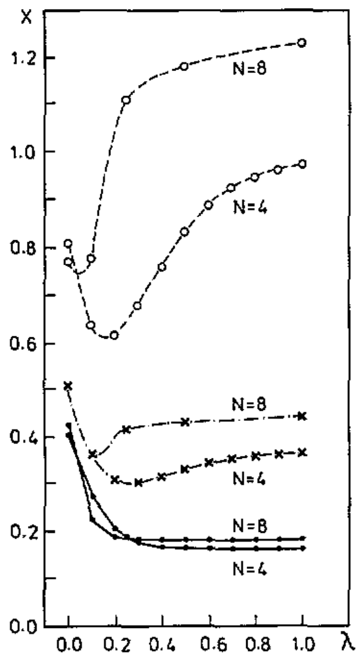

Figure 3. Scaling dimension of the $(3 \times \frac{1}{2})$ model. Full circles (●) denote the singlet–triplet values, open circles (○) the singlet–singlet values, and crosses (×) the linear combination (2.4) of the two. The lines are guides for the eye.

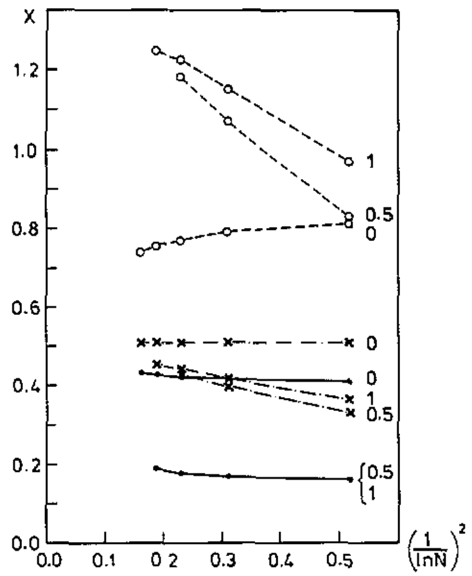

Figure 4. Scaling against $(\ln N)^{-2}$ of the scaling dimension of the $(3 \times \frac{1}{2})$ model. Symbols are the same as in figure 3. The numbers on the right refer to the values of λ. The non-monotronic behaviour with respect to λ is in accordance with figure 3.

We still have to prove, however, that the numerical analysis we have made is accurate enough to make possible a clear distinction between critical and non-critical models. To this end we have made the same analysis for the $(2 \times \frac{1}{2})$ model which interpolates between the $S = \frac{1}{2}$ and $S = 1$ Heisenberg chains. We describe next our results for the $(2 \times \frac{1}{2})$ model of a quantity which would be the central charge if it existed.

The spin wave velocity of the $(2 \times \frac{1}{2})$ model is determined in the same way as that of the $(3 \times \frac{1}{2})$ model. Therefore we will find the correct velocity if there is no gap in the excitation spectrum at $k = 0$. We find that

$$v(\lambda) = \tfrac{1}{2}\pi + 2.5127\lambda - 0.3333\lambda^2. \tag{3.2}$$

In figure 5 we show the central charge (if it exists) for the $(2 \times \frac{1}{2})$ model as a function of λ for various N. This is calculated in the same way as figure 1 for the $(3 \times \frac{1}{2})$ model. The most obvious difference is that in figure 5 there does not appear to be a region over which c is effectively constant. The value of c in the limit $N \to \infty$ appears to be small except at $\lambda = 0$. To investigate this further we show in figure 6 a plot of c as a function of $(\ln N)^{-3}$ which is the expected form of the correction to the N^{-2} scaling of $E_0(N)$ if the model is critical and is in the same universality class as the $S = \frac{1}{2}$ Heisenberg chain. This figure shows rather clearly the difference in the limiting values for $\lambda = 0$ and $\lambda \neq 0$, and should be compared with figure 2.

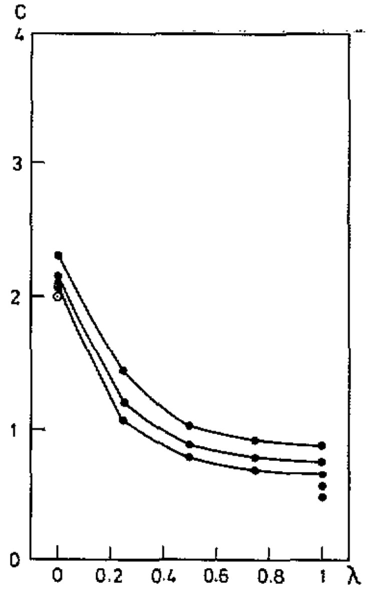

Figure 5. 'Central charge' of the $(2 \times \frac{1}{2})$ model which has been calculated in the same way as that of the $(3 \times \frac{1}{2})$ model. The curves from top to bottom are the results for $N = 4$, 6 and 8, respectively. The results for $N = 10$ and 12 are shown only for $\lambda = 1$, and the expected limiting value is marked for $\lambda = 0$.

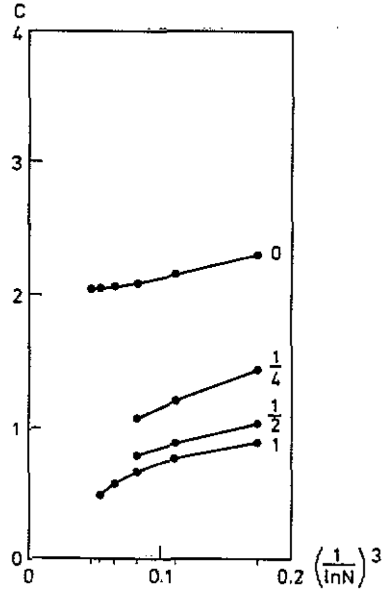

Figure 6. Scaling against $(\ln N)^{-3}$ of the 'central charge' of the $(2 \times \frac{1}{2})$ model. Symbols are the same as in figure 2.

4. Discussion

We have studied in this paper the finite size scaling properties of the ground state and the first few excited states of the $(2 \times \frac{1}{2})$ model and $(3 \times \frac{1}{2})$ model. These models interpolate between the $S = \frac{1}{2}$ Heisenberg chain and the $S = 1$ and $S = \frac{3}{2}$ Heisenberg chains, respectively. Our analysis complements that of Ziman and Schulz [11] whose model interpolates between the integrable $S = \frac{3}{2}$ model and the $S = \frac{3}{2}$ Heisenberg chain. Another aspect of our analysis is to estimate the usefulness of the numerical determination of the central charge and the scaling dimension as test of critical behaviour.

Our results for the $(3 \times \frac{1}{2})$ model strongly support the conjecture we have made earlier [9, 14] that, whenever $\lambda > 0$, the model behaves rather like the $S = \frac{3}{2}$ Heisenberg chain. This conclusion is suggested by the scaling of the $S = \frac{3}{2}$ like plateau in figure 1. Our numerical findings lend also strong support to the conclusion that the central charge of the $(3 \times \frac{1}{2})$ model is $c = 1$ (for all $\lambda > 0$), and its scaling dimension is $X = \frac{1}{2}$ [17]. Furthermore, these quantities seem to scale as a function of N in accordance with the leading logarithmic corrections to the corresponding quantities of the $S = \frac{1}{2}$ Heisenberg chain [18].

As to our numerical findings for the $(2 \times \frac{1}{2})$ model, they also provide evidence for twofold conclusions. Firstly, for any $0 < \lambda \leqslant 1$ the behaviour of the model is similar to that of the $S = 1$ Heisenberg chain. Secondly, the quantity defined as the central charge does not have a well defined meaning for this model except at $\lambda = 0$, as it appears to vanish for any non-zero λ. If the central charge were meaningful for this model, one might expect it to be either $c = 1$, i.e. the same as for the $S = \frac{1}{2}$ Heisenberg chain, or $c = 1.5$ which is the value for the integrable $S = 1$ Hamiltonian [19]. Our numerical results rule out both of these values. As a further check on the possible criticality of the $(2 \times \frac{1}{2})$ model we have studied the scaling of the central charge as a function of $(\ln N)^{-3}$. With a proviso due to the relative shortness of the chains we can treat numerically, the scaling is satisfied only by the $\lambda = 0$ result.

Summing up the results we have reported in this paper, we can conclude that even in numerical studies, central charge and scaling dimension are good indicators of criticality. In the determination of the scaling dimension it is crucial to use the method of linear combination of the singlet–triplet and singlet–singlet gaps first introduced in [11]. Otherwise the leading logarithmic corrections to the finite size results will mask the true asymptotic behaviour even for relatively long chains [13].

Our results also lend further support to our previous findings [9, 14] that in the limit $N \to \infty$ the composite $(n \times \frac{1}{2})$ models behave like the $S = \frac{n}{2}$ Heisenberg chains for all $\lambda > 0$. On the other hand, the methods used in this work seem to distinguish the properties of integer spin Heisenberg chains from those of half-integer spin Heisenberg chains better than was possible by using only the lowest gaps to excitations [9, 14]. The gaps alone, at least for numerically accessible chain lengths, did not provide [9, 14] conclusive evidence for either criticality or non-criticality of the isotropic antiferromagnetic point of the Heisenberg chain.

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[19] Affleck I 1986 *Phys. Rev. Lett.* **56** 746–8