Critical behaviour of spin-s Heisenberg antiferromagnetic chains: analytic and numerical results

1989 J. Phys. A: Math. Gen. 22 511

(http://iopscience.iop.org/0305-4470/22/5/015)

J. Phys. A: Math. Gen. **22** (1989) 511-529. Printed in the UK

Critical behaviour of spin-s Heisenberg antiferromagnetic chains: analytic and numerical results

Ian Affleck†, Doron Gepner‡, H J Schulz§ and Timothy Ziman‖

† Canadian Institute for Advanced Research and Physics Department, University of British Columbia, Vancouver, BC, Canada V6T 2A6

‡ Joseph Henry Laboratories, Princeton University, Princeton, NJ 08544, USA

§ Laboratoire de Physique des Solides, Universite de Paris-Sud, 91405 Orsay, France

‖ Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08855, USA

Received 28 June 1988

Abstract. A general phase diagram for isotropic antiferromagnetic chains has been proposed recently, using conformal field theory. This is developed further to predict the spectrum of finite chains, including logarithmic corrections. These predictions are tested against Bethe ansatz and exact diagonalisation results for various Hamiltonians with $s=\frac{1}{2}$, 1 and $\frac{3}{2}$. Logarithmic corrections to correlation functions and the scaling of gaps for infinite systems are also given.

1. Introduction and conclusions

Recent developments in conformal field theory have led [1-3] to a rather complete phase diagram for isotropic antiferromagnetic chains of arbitrary spin s. The set of all minimal isotropic critical theories is given by the Wess-Zumino-Witten (wzw) non-linear σ models with topological coupling constant k, a positive integer [1]. The only stable critical point is $k=1$, which corresponds to a free boson. This is an attractive fixed point for a range of half-odd-integer-s Hamiltonians [2, 3]. Integer-s Hamiltonians generally show non-universal behaviour with a gap [4]. The higher-k theories represent multicritical points which can be attained by adjusting one or more parameters in the spin Hamiltonian. In particular, the Bethe ansatz integrable spin-s Hamiltonian [5-7] is attracted to the $k=2s$ multicritical point.

In this paper we will help to verify this picture by comparing the field theory predictions to other exact theoretical results on the spectrum of finite chains. These are of three types. We present results of exact diagonalisation of $s=\frac{1}{2}$ chains of length 20. We also present numerical results obtained using the Bethe ansatz for solvable Hamiltonians with $s=\frac{1}{2}$, 1 and $\frac{3}{2}$. While the solvable $s=\frac{1}{2}$ Hamiltonian is just the conventional Heisenberg model, the $s=1$ Hamiltonian contains both bilinear and biquadratic $[(\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1})^2]$ terms and the $s=\frac{3}{2}$ Hamiltonian contains bilinear, biquadratic and bicubic terms. We present results for chains of length up to 2048, 256 and 100 for these models with $s=\frac{1}{2}$, 1 and $\frac{3}{2}$ respectively. Finally we compare our results with the *analytic* Bethe ansatz expressions of Woynarovich and Eckle [8] for the first few corrections in $1/L$ to the energies.

These data can be used to test the proposed phase diagram [2, 3] because the scaling of energies with length, L, shows a universal behaviour determined by the

0305-4470/89/050511+19$02.50

critical theory. In general, in a conformally invariant theory the energy levels form towers of the form

$$E - E_0 = (2\pi v/L)(x+n) \tag{1}$$

where E_0 is the ground-state energy, v is the velocity of 'light', n is an arbitrary positive integer and x is the scaling dimension of a primary field [9]. A tower of this kind appears for each primary field. Thus the complete set of critical exponents can be determined from the finite-size spectrum. For a system which is not exactly conformally invariant, but only asymptotically so at low energies, there are corrections to this formula which vanish more rapidly as $L \to \infty$. They can be associated with irrelevant operators in the Hamiltonian describing the system [10]. An operator with dimension $2+a$ leads to corrections proportional to $1/L^{1+a}$. Marginally irrelevant variables produce logarithmic corrections, $x \to x + d/\ln L$, in (1), where d is a universal number, determined by β function coefficients, or equivalently three-point functions [11]. Corrections to the ground-state energy of $O(1/L)$ and $O[1/L(\ln L)^3]$ are also universal [11-13].

The exact values of all these parameters will be obtained here from the wzw theories and the predictions compared with exact Bethe ansatz and numerical finite-chain results. The logarithmic terms normally imply that finite-chain convergence is extremely slow; the next correction is only down by an additional power of $1/\ln L$. This normally makes it very difficult to probe the critical behaviour. This can be seen rather clearly in our Bethe ansatz results on long chains. We get around this problem, for a particular Hamiltonian of only 20 sites, in a way first exploited by Jullien and Haldane [14]†. Since there is only one marginal operator we should be able to change its coupling constant by varying any parameter in the underlying microscopic Hamiltonian. We consider a nearest-neighbour plus second-nearest-neighbour $s = \frac{1}{2}$ chain and vary the ratio of the two couplings. We find a special value of this ratio where the log corrections vanish and excellent agreement with the analytic predictions are obtained from a chain of only 20 sites.

On the whole these comparisons suggest that the various calculations are consistent. The agreement between numerical and analytic results is particularly striking for the short $s = \frac{1}{2}$ chain with vanishing log corrections and the integrable (Heisenberg) $s = \frac{1}{2}$ chains with length up to 2048. The agreement for the shorter $s = 1$ and $\frac{3}{2}$ solvable chains is not as good, but probably reasonable considering the modest lengths and the log corrections. The agreement with the analytic Bethe ansatz formulae is exact except for an unexplained discrepancy in one dimensionless coefficient.

The general formula for the excitation energies with logarithmic corrections was first given in [15]. The excitation energies for the $s = \frac{1}{2}$ case were derived in [16] and for the related Potts model in [17]. Bethe ansatz results were compared with conformal field theory predictions for the $s = \frac{1}{2}$, 1, $\frac{3}{2}$ and 2 case in [18]. Other related results were obtained in [19].

In the next section we review the proposed critical theories. In § 3 we derive formulae for the finite-chain spectrum. The *multiplicative* logarithmic corrections to correlation functions and to the scaling of infinite-L gaps upon adding relevant operators are determined by the same renormalisation group coefficients that determine the log corrections to the finite-L scaling in the gapless phase. In § 4 we derive these log corrections to the correlation function and the log correction to the scaling of the

† Haldane has shown (in his 1988 letter [14]) that even greater degeneracies occur with a $1/r^2$ interaction.

gap upon moving away from the integrable point for the $s=1$ bilinear-biquadratic model or upon adding an alternating interaction for half-odd-integer s. In § 5 we compare our field-theoretical predictions with exact diagonalisation of finite $s=\frac{1}{2}$ chains and in § 6 with Bethe ansatz results.

2. The critical theory

The approach to quantum spin chains used in [3] is based on the strong-coupling limit of the Hubbard model, and its multiband generalisation to obtain higher s. The analysis of these models is in fact based on the *weak-coupling* limit. The basic idea is to separate the gapless spin excitations from the charge excitations which have a gap (for $s>\frac{1}{2}$, additional types of excitations also occur, associated with the 'colour' quantum numbers describing the various bands). Renormalisation group and universality ideas suggest that the only effect of going from weak to strong coupling is to increase the gap for the charge (and colour) excitations; the effective low-energy theory describing the gapless spin excitations is unchanged. This separation of spin excitations from charge (and colour) is achieved by bosonisation. In [1, 3] non-Abelian bosonisation [20] was used in order to keep manifest the isotropy of the problem, which tends to be concealed by the more conventional Abelian bosonisation.

Before briefly reviewing the essential results of bosonisation, we examine the symmetries of the non-interacting electron gas. The tight-binding model is written

$$H = t \sum_i (\psi_i^{\alpha +} \psi_{i+1,\alpha} + \text{HC})$$

where the repeated spin index α is summed over $\uparrow$ and $\downarrow$ and HC stands for Hermitian conjugate. This model has charge and spin symmetries

$$\psi_\alpha \to \mathrm{e}^{i\theta} \psi_\alpha$$

$$\psi_\alpha \to U_\alpha^\beta \psi_\beta$$

where U_α^β is an SU(2) matrix, and repeated spin indices are summed. Taking the continuum limit for a half-filled band we obtain independent left- and right-moving electrons, with Hamiltonian density

$$H/v = \psi_{\mathrm{L}}^{+\alpha}(\mathrm{i}\,\mathrm{d}/\mathrm{d}x)\psi_{\mathrm{L}\alpha} - \psi_{\mathrm{R}}^{+\alpha}(\mathrm{i}\,\mathrm{d}/\mathrm{d}x)\psi_{\mathrm{R}\alpha}.$$

(Here $v=2t$ is the Fermi velocity.) This model has *chiral* charge and spin symmetries under which the left and right electrons transform independently. In other words the charge and spin of left- and right-moving electrons are separately conserved.

The Hubbard-model interaction introduces terms, among others, of the form $\varepsilon_{\alpha,\beta}\psi_{\mathrm{L}}^{\alpha +}\psi_{\mathrm{L}}^{\beta +}\psi_{R\gamma}\psi_{\mathrm{R}\delta}\varepsilon^{\gamma\delta}$ (where $\varepsilon_{\alpha,\beta}$ is the antisymmetric tensor and repeated indices are summed) which break the chiral symmetries down to the diagonal subgroup under which the left- and right-moving electrons transform identically. Thus the continuum model has no more charge or spin symmetry than the lattice model. The Hubbard-model Hamiltonian and some of its generalisations, which describe higher-spin systems, flow to fixed points under renormalisation group transformations. It is a remarkable fact that in all cases these fixed-point Hamiltonians have the chiral spin symmetry of the non-interacting fermions (although the Hamiltonian is not the same). This was shown

in [1]. Essentially the conformal invariance of a fixed point is only compatible with chiral symmetries, not purely diagonal symmetries.

It follows that the energy levels of the conformal field theory describing the fixed point can all be classified by two different spin quantum numbers, $\boldsymbol{S}_L$ and $\boldsymbol{S}_R$, just as is the case for the continuum non-interacting electron model. The total spin is just the sum

$$\boldsymbol{S} = \boldsymbol{S}_L + \boldsymbol{S}_R .$$

Only the total spin is an exactly conserved quantity of the quantum spin chain. The separate left and right spins can only be used to classify the low-energy states, which are described by the fixed-point Hamiltonian. This means that there are irrelevant operators in the Hamiltonian which break the higher chiral symmetry. However, these make contributions to the energies which become negligible for $L \to \infty$.

The various possible critical points which may occur can be conveniently classified by their current algebras [21]. The generators of left and right SU(2) rotations of the non-interacting fermion model are

$$\boldsymbol{J}_{L,R} = \psi^{+\alpha}_{L,R} \tfrac{1}{2} \boldsymbol{\sigma}^{\beta}_{\alpha} \psi_{L,R\beta}$$

where the σ^a are Pauli matrices. The three components of $\boldsymbol{J}_L$ obey commutation relations known as the Kac-Moody algebra. There is a normalisation parameter in this algebra known as the Kac-Moody central charge, k, which is always an integer. For the non-interacting fermion model, it is equal to the number of colours, and so $k = 1$ for the ordinary Hubbard model. The minimal conformal field theory (with the smallest spectrum) containing currents obeying the Kac-Moody algebra with central charge k is the Wess-Zumino-Witten non-linear σ model (wzw model), with topological coupling constant k. A complete classification of primary fields and of the spectrum has been performed for these models [22]. These operators can be classified according to their left and right spin. There is one operator with $s_L = s_R = 0, \frac{1}{2}, \ldots, k/2$. Its scaling dimension is

$$x = 2s_L(s_L + 1)/(2 + k).$$

The operators with s_L half-odd integer (integer) are odd (even) under translation by one site; thus they correspond to states with momentum near π (zero). Because we are considering translationally invariant spin chains, only the integer s_L operators can be generated in the effective Hamiltonian. We note that for $k = 1$ there are no permitted relevant operators (the $s_L = 0$ field is the identity) and for $k = 3$ there is one relevant operator with $s_L = 1$, $x = \frac{4}{5}$.

In addition to these relevant operators there is a very important marginal operator for all k, namely $\boldsymbol{J}_L \cdot \boldsymbol{J}_R$. (It is not a primary field of the Kac-Moody algebra.) This will be marginally relevant or irrelevant depending on the sign of the coupling constant. While the coupling constant has the irrelevant sign for the nearest-neighbour Heisenberg model, it can be made to pass through zero and change sign by adding a second-nearest-neighbour interaction. The $k = 1$ wzw model is the only stable critical point, and describes the generic gapless phase for half-integer-s chains. The integrable spin-s chain flows to the $k = 2s$ multicritical point. Perturbing the Hamiltonian will in general induce flow away from this critical point to the $k = 1$ point, for half-integer s or to non-universal short-range behaviour for integer s.

3. Spectrum

3.1. O(1/L) terms

The spectrum of a general conformal field theory mimics the separation into left and right movers observed above in the non-interacting electron model. The left and right components of the energy-momentum tensor, $P_{L,R}$, give $\pm$ the momentum and $1/v$ times the energy of the left (right) movers. Thus the momentum and energy are given by

$$P = P_L - P_R \tag{2a}$$

$$E = v(P_L + P_R). \tag{2b}$$

In general, primary fields have a left and right scaling dimension $x_{L,R}$, with the sum being the dimension x discussed above. The conformal towers are obtained by applying raising operators to the primary states. The towers are classified by two integers $n_{L,R}$, the single integer, n, discussed above being the sum

$$P_{L,R} = (2\pi/L)(x_{L,R} + n_{L,R}).$$

The wzw models have [22] primary fields of dimension $x_L = x_R = s_{L0}(s_{L0}+1)/(2+k)$, with $s_{L0} = s_{R0} = \frac{1}{2}, 1, \ldots, k/2$ being the left and right spin. These will correspond to the lowest states in the conformal towers. Since the primary fields with half-integer s_{L0} are odd under translation by one site, the corresponding lowest states have momentum π and for these states equation (2*a*) becomes

$$P = P_L - P_R + \pi.$$

In general the raising operators are just Fourier modes of the energy-momentum tensor. In conformal field theories with conserved currents, the Fourier modes of the currents can also be used as raising operators. In the SU(2)-invariant case there are raising operators which raise P_L and also S_L^z or P_R and S_R^z by one or more units. Thus a general level in a conformal tower is classified by n_L, n_R, s_L, s_R, S_L^z and S_R^z (with $s_L \geqslant s_{L0}$, $s_R \geqslant s_{R0}$). To complete the specification of the conformal towers we must give the multiplicity of each level.

The representations of ordinary SU(2) can be found by starting with some state with some assumed quantum numbers, $|s, S^z\rangle = |s, -s\rangle$, making the assumption $S^-|s, -s\rangle = 0$ (in order to get a finite-dimensional representation) and then applying S^+ using the commutation relations and the condition $\boldsymbol{S}^2 = s(s+1)$. A similar construction can be performed for the Kac-Moody algebra. We begin with the lowest states in a conformal tower of spin $s_{L0} = s_{R0}$, which have multiplicity one, $S_L^z = -s_{L0}, -s_{L0}+1, \ldots, s_{0L}$ and $S_R^z = -s_{R0}, -s_{R0}+1, \ldots, s_{R0}$. We apply raising operators to generate the complete tower. Because the left and right currents commute, we may calculate the left conformal tower separately, giving a set of multiplicities m_L as a function of n_L, s_L and S_L^z. The same tower is obtained using the right raising operators. The multiplicity of a state in the combined conformal tower is then

$$m = m_L(n_L, s_L, S_L^z) m_R(n_R, s_R, S_R^z).$$

It turns out to be more convenient to specify multiplicities as a function of n_L and S_L^z only; a unique classification into SU(2) multiplets such that $S_L^z = -s_L, -s_L+1, \ldots, s_L$ is then determined. The left-handed conformal tower can be constructed, beginning

from the lowest level with some specified spin s_{L0}, using three rules which follow from the Kac-Moody algebra.

(i) $m(n_L, S_L^z) = m(n_L, -S_L^z)$.

(ii) Starting from any state with some value of n_L, $S_L^z > 0$, follow the diagonal line in the n_L, S_L^z diagram to the point $-S_L^z - k$, $n_L + 2S_L^z + k$. This point has the same multiplicity. All points in between have non-zero multiplicity, but all points further along the diagonal (at larger n_L) have multiplicity 0.

These rules determines the shape of the conformal tower in the n_L, S_L^z diagram. This shape is drawn in figure 1 for $k=1$ and $k=3$, for the conformal towers with $s_{L0} = s_{R0} = 0$. This shape determines the susceptibility. To see this note that the envelope of the conformal tower of spin s_L, is given by the states with

$$S_L^z = \pm(s_{L0} + pk) \qquad n_L = 2ps_{L0} + p^2 k \qquad p = 0, 1, 2, \ldots .$$

This envelope is the parabola

$$n_L = [(S_L^z)^2 - (s_{L0})^2]/k. \tag{3}$$

To calculate the susceptibility, we add an external field h to H. This shifts the energy of an arbitrary state as

$$E \to E_0 + (2\pi v/L)(x + n_L + n_R) - h(S_L^z + S_R^z).$$

Taking the limit of large L *before* taking $h \to 0$, we may approximate $n_{L,R}$ by their values on the envelope of the conformal tower for large S^z

$$E \approx E_0 + (2\pi v/Lk)[(S_L^z)^2 + (S_R^z)^2] - h(S_L^z + S_R^z).$$

We now minimise E with respect to $S_{L,R}^z$ giving

$$S_{L,R}^z = h(Lk/4\pi v)$$

$$E(h) = E_0 - \tfrac{1}{2}h^2(Lk/2\pi v).$$

Thus the susceptibility is

$$\chi \equiv -\mathrm{d}^2 E/\mathrm{d}h^2 = Lk/2\pi v.$$

This, of course, agrees with the result derived earlier [23] by expressing χ in terms of the current two-point function.

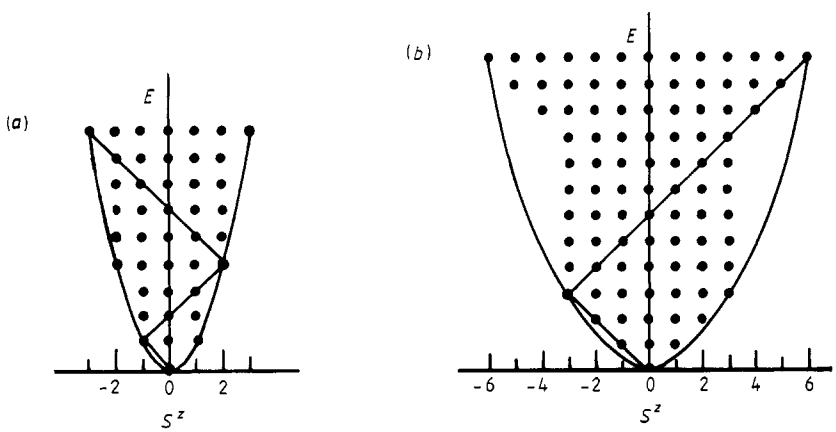


Figure 1. The shape of the Kac-Moody conformal towers for: (*a*) $k=1$, $s_{L0} = s_{R0} = 0$; (*b*) $k=3$, $s_{L0} = s_{R0} = 0$.

(iii) The non-zero multiplicities are determined as follows. All states reached from the lowest states by the construction of rule (i) have $m=1$. For each value of (S_L^z, n_L) for which m is non-zero, as determined by rule (i), the following equation holds:

$$\sum_{j=-\infty}^{\infty}(-1)^j m[S_L^z-j,\ n-j(j+1)/2]=0.$$

The sum may be restricted to the states of non-zero m as determined by rule (i) (in particular, terms with $[n-j(j+1)/2]<0$ may be dropped). Thus there is a finite number of terms for each value of (S_L^z, n_L).

The first few levels of the two left conformal towers for $k=1$ (with $s_{L0}=0$ or $s_{L0}=\frac{1}{2}$), and the four left conformal towers for $k=3$ (with $s_{L0}=0, \frac{1}{2}, 1, \frac{3}{2}$) are shown in table 1. We give the degeneracies of complete spin multiplets, rather than states of definite S_L^z.

The $k=1$ theory is equivalent to a free boson, with Lagrangian

$$L=\tfrac{1}{2}\partial_\mu\varphi\partial^\mu\varphi$$

and periodicity condition

$$\varphi(x+L)=\varphi(x)+\sqrt{2\pi}n$$

Table 1. Degeneracies of s_L multiplets.

	$k=1,\ s_{L0}=0$			$k=3,\ s_{L0}=\frac{1}{2}$			
n_L	$s_L=0$	$s_L=1$	$s_L=2$	$s_L=\frac{1}{2}$	$s_L=\frac{3}{2}$	$s_L=\frac{5}{2}$	$s_L=\frac{7}{2}$
5	2	4	1	12	14	8	2
4	2	2	1	7	8	4	1
3	1	2		4	4	2	
2	1	1		2	2	1	
1	0	1		1	1		
0	1			1			

	$k=1,\ s_{L0}=\frac{1}{2}$		$k=3,\ s_L=1$				
n_L	$s_L=\frac{1}{2}$	$s_L=\frac{3}{2}$	$s_L=0$	$s_L=1$	$s_L=2$	$s_L=3$	$s_L=4$
5	4	3	8	16	14	5	1
4	3	2	4	10	7	3	
3	2	1	3	5	4	1	
2	1	1	1	3	2		
1	1		1	1	1		
0	1		0	1			

	$k=3,\ s_{L0}=0$				$k=3,\ s_L=\frac{3}{2}$			
n_L	$s_L=0$	$s_L=1$	$s_L=2$	$s_L=3$	$s_L=\frac{1}{2}$	$s_L=\frac{3}{2}$	$s_L=\frac{5}{2}$	$s_L=\frac{7}{2}$
5	3	9	6	3	10	12	7	2
4	3	4	4	1	6	7	4	1
3	1	3	1	1	3	4	2	
2	1	1	1		2	2	1	
1	0	1			0	1		
0	1				0	1		

where n is an integer. In this case, as can be easily checked, the lowest states of given integer s_L or s_R *all* lie on the envelope of the $s_{L0} = s_{R0} = 0$ conformal tower and hence obey the equation

$$E - E_0 = (2\pi v/L)[(s_L)^2 + (s_R)^2]. \tag{4}$$

States with half-odd-integer $s_{L,R}$ lie on the other conformal tower with $s_{L0} = s_{R0} = \frac{1}{2}$. Again all lowest states of given $s_{L,R}$ lie on the envelope, this time obeying $n_L = s_L^2 - \frac{1}{4}$. Since $x = \frac{1}{2}$ the energies of these states also obey equation (4).

We present calculations below for states with momentum 0 or π. These states have $n_L = n_R = n/2$. The values of (s_L, s_R) for the first few levels of the $k = 1$ multiplets are shown in table 2. For each multiplet with definite values of s_L and s_R the total spin multiplets are determined by the usual rules for adding angular momentum: $s_T = s_L + s_R$, $s_L + s_R - 1, \ldots, |s_L - s_R|$. The degeneracies of the multiplets of given total spin as a function of the scaled energy gap, $L(E - E_0)/2\pi v$ are given in table 3 for $k = 1$. Very large degeneracies set in as n increases, which are entirely 'accidental' from the point of view of the symmetries of the spin chain. They are a consequence of the conformal and chiral symmetries of the critical theory.

Although the ground-state energy itself is not a universal quantity, the $O(1/L)$ correction *is* universal, being determined by the conformal anomaly parameter, c, which has the value

$$c = 3k/(2+k).$$

The ground-state energy has the form

$$E_0 = e_0 L - \pi c v/6L + \text{higher-order terms}.$$

One way of understanding this result is to realise that a field theory at zero temperature on a line of length L is equivalent to the same field theory at temperature v/L on an

Table 2. (s_L, s_R) multiplets for $k = 1$.

n	$P = 0$ ($s_{L0} = s_{R0} = 0$, conformal tower)	$P = \pi$ ($s_{L0} = s_{R0} = \frac{1}{2}$, conformal tower)
4	(1, 1), (1, 0), (0, 1), (0, 0)	$(\frac{3}{2}, \frac{3}{2})$, $(\frac{3}{2}, \frac{1}{2})$, $(\frac{1}{2}, \frac{3}{2})$, $(\frac{1}{2}, \frac{1}{2})$
2	(1, 1)	$(\frac{1}{2}, \frac{1}{2})$
0	(0, 0)	$(\frac{1}{2}, \frac{1}{2})$

Table 3. Degeneracies of total spin multiplets for $k = 1$.

	$P=0$				$P=\pi$			
$[(L/2\pi v)(E - E_0)]$	$s=0$	$s=1$	$s=2$	$s=3$	$s=0$	$s=1$	$s=2$	$s=3$
$\frac{9}{2}$					2	4	3	1
4	2	3	1					
$\frac{5}{2}$					1	1		
2	1	1	1					
$\frac{1}{2}$					1	1		
0	1							

infinite line. The ground-state energy is then equivalent to the free energy per unit length divided by the product of temperature and velocity:

$$f/T = e_0/T - \pi c T/6v$$

implying a linear specific heat,

$$c(T) = \pi c T/3v.$$

The slope of the specific heat measures the density of states and is thus a universal number. Indeed the specific heat can be related to the two-point correlation function of the Hamiltonian, which is proportional to the conformal anomaly parameter, c.

3.2. 1/L ln L terms

The degeneracies of the excited states are broken by the finite-size corrections which vanish more rapidly than $1/L$. These are a consequence of irrelevant operators in the effective Hamiltonian which do not respect the full conformal and chiral symmetry, but only the exact symmetries of the spin chain, namely the diagonal SU(2) subgroup and the lattice symmetries. These higher-order corrections can be calculated in first-order perturbation theory in the irrelevant operators, replacing the coupling constants by their renormalised values at scale L. Thus irrelevant operators of dimension $2+d$ give corrections to the energies of $O(1/L^{1+d})$.

Marginal operators give corrections which are only suppressed by an additional logarithm [11, 13]. If we write the marginal operator in the Hamiltonian as

$$\delta H = g \int \mathrm{d}x\, \varphi$$

then the perturbation to the excitation energy of a state $|\varphi_i\rangle$ is

$$\delta(E_i - E_0) = g \int \mathrm{d}x \langle \varphi_i | \varphi(x) | \varphi_i \rangle \equiv g b_i (2\pi)^2 / L \tag{5}$$

where the matrix element can be conveniently expressed in terms of the three-point function involving the marginal operator and the operator φ_i which corresponds to the state $|\varphi_i\rangle$. (In conformal field theory there is an operator corresponding to each state.) In what follows we assume that φ and φ_i are primary fields with respect to the Virasoro algebra, with $x_L = x_R$. In general higher states in the Kac-Moody conformal towers are obtained from the bottom state by applying Fourier modes of J_L *and* Fourier modes of T_L. In what follows, the states $|\varphi_i\rangle$ are assumed to be obtained by applying Fourier modes of J_L *only*. While it is not immediately obvious exactly which states these are, they certainly include the lowest-energy multiplet with any given quantum numbers $s_{L,R}$, since applying Fourier modes of $T_{L,R}$ always raises the energy without changing the spin. The second assumption, $x_L = x_R$ implies that the states have momentum 0 or π. Normalising the operators to have two-point functions

$$\langle 0 | \varphi_i(r_1) \varphi_i(r_2) | 0 \rangle = |r_1 - r_2|^{-2x}$$

the coefficient b_i can be determined from the three-point function as

$$\langle 0 | \varphi_i(r_1) \varphi(r_2) \varphi_i(r_3) | 0 \rangle = -b_i / (|r_{12}|^2 |r_{23}|^2 |r_{13}|^{2x-2}). \tag{6}$$

Equation (5) can be 'renormalisation group improved' by replacing g by $g(L)$ the effective coupling at scale L [11]. If g is initially small, the one-loop β function gives

$$g(L) = g/(1 + \pi b g \ln L/L_0) \tag{7}$$

where b is again determined by a three-point function

$$\langle 0|\varphi(r_1)\varphi(r_2)\varphi(r_3)|\rangle = -b(|r_{12}|^2|r_{23}|^2|r_{13}|^2)$$

and L_0 is the scale at which the bare coupling g is determined (essentially the lattice spacing). We have defined the sign of the marginal operator, φ, so that the term is marginally irrelevant for $g > 0$. At very large L, $g(L)$ becomes independent of its starting value

$$g(L) \to 1/\pi b \ln L$$

giving a universal logarithmic correction to the energy

$$\delta(E_i - E_0) = 4\pi v b_i / bL \ln L.$$

This asymptotic form of $g(L)$ holds even if g is not initially small. In general, $\ln L$ must be much greater than 1 before this asymptotic expression for $g(L)$ holds. If g is initially small then $g(L)$ will be essentially constant out to enormously large L. Also note that second-order perturbation theory would give terms proportional to $g(L)^2$ and hence only suppressed by one extra power of $\ln L$.

Hence from a practical point of view, the universal asymptotic expression is not very useful for studying numerical results for relatively small systems. However, (5) *is* useful when g is small. Although it will not be possible to predict the precise value of g in general, (5) predicts the *relative* size (and sign) of the corrections to all energy levels corresponding to primary fields with respect to the Virasoro algebra. By varying a parameter in the microscopic Hamiltonian one can arrange to sit close to the critical point where the marginal operator is absent. In general g should grow linearly as an arbitrary parameter is varied in the microscopic Hamiltonian which moves the critical theory away from the fixed point.

The coefficients b_i which determine the shifts of the energy levels due to the marginal operator take a particularly simple form for isotropic spin chains. Let us consider the matrix elements of the marginal operator $\boldsymbol{J}_L \cdot \boldsymbol{J}_R$ in the states in some multiplet of definite s_L and s_R. This is proportional to $\boldsymbol{S}_L \cdot \boldsymbol{S}_R$, for the various states in the multiplet. This in turn is given by the total spin s, which takes on values between $s_L + s_R$ and $|s_L - s_R|$. Explicitly,

$$\begin{aligned}\boldsymbol{S}_L \cdot \boldsymbol{S}_R &= \tfrac{1}{2}[\boldsymbol{S}_L + \boldsymbol{S}_R)^2 - \boldsymbol{S}_L^2 - \boldsymbol{S}_R^2] \\ &= \tfrac{1}{2}[s(s+1) - s_L(s_L+1) - s_R(s_R+1)].\end{aligned}$$

We may easily relate the magnitudes of the splittings between different multiplets. This follows from (6), which relates the matrix element of $\boldsymbol{J}_L \cdot \boldsymbol{J}_R$ to the three-point function involving $\boldsymbol{J}_L \cdot \boldsymbol{J}_R$ and the primary field corresponding to the state in question. This three-point function is determined by the operator product expansion coefficient involving $\boldsymbol{J}_L$ (or $\boldsymbol{J}_R$) and the primary field

$$\boldsymbol{J}_L(z)\varphi_i(z') = \boldsymbol{S}_L\varphi_i(z)/2\pi(z - z') + \ldots.$$

The universal coefficient of this operator product expansion follows from the fact that $\int \mathrm{d}x\, \boldsymbol{J}_L = \boldsymbol{S}_L$, a conserved charge. The current two-point function is determined by the Kac-Moody central charge as

$$\langle J_L^a(z) J_L^b(0)\rangle = \delta^{ab} k/(8\pi^2 z^2).$$

Thus the normalised marginal operator is

$$\varphi = -(8\pi^2/\sqrt{3}k)\boldsymbol{J}_L \cdot \boldsymbol{J}_R.$$

Since $\boldsymbol{J}_L$ and $\boldsymbol{J}_R$ commute, we immediately conclude that

$$b_i = -\boldsymbol{S}_L \cdot \boldsymbol{S}_R(2/\sqrt{3}k).$$

Thus the $O(1/L \ln L)$ shift in the energy is proportional to $\boldsymbol{S}_L \cdot \boldsymbol{S}_R$ with a constant of proportionality which is the same for all states which correspond to primary fields. Here primary field refers to the Virasoro algebra classification, not the Kac-Moody classification.

This formula also determines the renormalisation group coefficient, b, since $\boldsymbol{J}_L \cdot \boldsymbol{J}_R$ is itself a primary field (with respect to the Virasoro algebra) with quantum numbers $s_L = s_R = 1$, $s = 0$ and hence $\boldsymbol{S}_L \cdot \boldsymbol{S}_R = -2$, and

$$b = 4/\sqrt{3}k.$$

In fact there is actually a more straightforward derivation of b_i which makes it clear that (5) holds with b_i as given above, for *arbitrary states with* $P = 0$, not just primary states. Consider

$$\langle \varphi_i | \boldsymbol{J}_L(x) \cdot \boldsymbol{J}_R(y) | \varphi_i \rangle$$

for any state, $|\varphi_i\rangle$, with $P = 0$. This quantity must vanish at $L \to \infty$ by translation invariance and the fact that $\boldsymbol{J}_R$ and $\boldsymbol{J}_L$ are functions only of the independent light-cone coordinates, $x_\pm$. For finite L it can only have the form constant$/L^2$, as dictated by the dimension of $\boldsymbol{J}$. Noting that the integral over x and y gives $\boldsymbol{S}_L \cdot \boldsymbol{S}_R$, the product of conserved spin operators, we see that

$$\langle \boldsymbol{J}_L(x) \cdot \boldsymbol{J}_R(y) \rangle = \boldsymbol{S}_L \cdot \boldsymbol{S}_R / L^2.$$

This implies the same value of b_i obtained above.

Thus the excitation energies for $P = 0$ states, including log corrections, are

$$E_i - E_0 = (2\pi v/L)(x_i - \boldsymbol{S}_L \cdot \boldsymbol{S}_R / \ln L). \tag{8}$$

The marginal coupling also makes a correction of $O(g^3)$ to the $O(1/L)$ term in the ground-state energy,

$$E_0 \approx e_0 L - (\pi/6L)(c + 2\pi^3 b g^3).$$

For very large L, we may replace g by its universal renormalisation group improved value, (7), giving

$$E_0 \approx e_0 L - (\pi/6L)[3k/(2+k) + 3k^2/8(\ln L)^3]. \tag{9}$$

Again, for comparison with numerical work on chains of moderate length, only the first of these two formulae is likely to be useful. The shifts of all excitation energies as well as the shift of E_0 are predicted in terms of a single unknown coupling constant, g, in the region where g is small.

4. Other logarithmic corrections

The logarithmic corrections to the excitation energies correspond to corrections to the anomalous dimensions, x_i, of the primary fields. Therefore, these same coefficients,

$b_i/2b$, determine logarithmic corrections to correlation functions, and to the scaling of the gap when the relevant operator φ_i is added to the Hamiltonian, in the infinite-length system. For completeness we review the general form of these logarithmic corrections and give explicit formulae for some cases of current interest.

The $O(g)$ corrections to the scaling dimensions x_i that we discussed above are corrections to the anomalous dimensions of φ_i:

$$\gamma_i = x_i + b_i g 2\pi + O(g^2).$$

The correlation function

$$G_i(r) \equiv \langle \varphi_i(r)\varphi_i(0)\rangle$$

obeys a renormalisation group equation

$$[\partial/\partial(\ln r) + \beta(g)\partial/\partial g + 2\gamma_i(g)]G_i(r, g) = 0.$$

Here $\beta(g) = -\pi b g^2 + O(g^3)$. Working to first order in g we have

$$G_i(r) = G_i(r_0)\exp\left(-\int_{r_0}^{r} d(\ln r')2\gamma_i(r')\right)$$

$$\propto (1/r^{2x_i})\exp\left(-(b_i 4\pi)\int_{r_0}^{r} d(\ln r')g(r')\right).$$

At moderate values of r the exponent $2x_i$ will simply appear to be corrected by the non-universal quantity $b_i g 2\pi$ (assuming g is small), but at exponentially large distances, using (7) for $g(r)$, the asymptotic form is given by

$$G_i(r) \propto 1/[r^{2x_i}(\ln r)^{4b_i/b}].$$

Note that this is a multiplicative correction rather than an additive one as occurred in the finite-size energies. The higher-order terms in γ_i and β give additive corrections which are suppressed by additional powers of $1/\ln r$. As an application of this general result, let us consider the spin-spin correlation function $\langle \boldsymbol{S}(r)\cdot\boldsymbol{S}(0)\rangle$.

The continuum-limit representation of the spin operators is

$$\boldsymbol{S}(r) \propto (-1)^r \times \text{constant} \times \text{Tr}\, g\boldsymbol{\sigma}$$

where we have kept only the staggered part of $\boldsymbol{S}$ which dominates at large separation. The primary field g has $s_L = s_R = \frac{1}{2}$, and the operator, Tr $g\boldsymbol{\sigma}$ has total spin, $s_T = 1$; thus

$$2b_i/b = -\tfrac{1}{4}$$

and

$$\langle \boldsymbol{S}(r)\cdot\boldsymbol{S}(0)\rangle \propto (-1)^r(\ln r)^{1/2}/r$$

for the $k = 1$ critical theory describing generic gapless half-odd-integer-s systems. For general k the $\ln r$ factor is the same but the exponent of $1/r$ becomes $3/(2+k)$.

Another situation in which logarithmic corrections arise is in calculating the scaling of a gap (for the infinite system) with the coefficient of a relevant operator which is added to the Hamiltonian. The correlation length ξ, which is proportional to the inverse gap, is the scale at which the effective coupling becomes $O(1)$. The β function for the relevant operator, including the term linear in g, is

$$dg_i/d(\ln L) = (2 - x_i)g_i - 2\pi b_i g g_i.$$

Integrating, and using the asymptotic form for $g(L)$, we find

$$\ln g_i(L)/g_i = (2-x_i)\ln L - (2b_i/b)\ln(\ln L) + \text{constant}$$

where g_i is the bare value of the relevant coupling, at the cutoff scale, L.

Setting $g_i(\xi) = 1$, we find

$$1/g_i \propto \xi^{2-x_i}/(\ln \xi)^{2b_i/b}.$$

Thus, the mass gap, m, scales as

$$m(g_i) \propto g_i^{1/(2-x_i)}/|\ln g_i|^{2b_i/b(2-x_i)}.$$

We consider two applications of this formula of current interest. One is the logarithmic correction to the spin-Peierls exponent. An alternating interaction

$$H \to \Sigma_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}[1+(-1)^i\alpha]$$

introduces the relevant operator Tr g into the continuum-limit Hamiltonian. (Tr g is normally not permitted because it is odd under the symmetry $g \to -g$, which corresponds to translation by one site.) This operator has $s_L = s_R = \frac{1}{2}$ and $s_T = 0$, and so

$$2b_i/b = \tfrac{3}{4}.$$

The dimension is $x = 3/2(2+k) = \frac{1}{2}$ for $k = 1$. Thus

$$m \propto \alpha^{2/3}/|\ln \alpha|^{1/2}$$

(for generic half-odd-integer-spin systems). For the $s = \frac{1}{2}$ case this agrees with the result derived previously [24].

Our second example involves the $k = 2$ multicritical point which occurs for the Bethe ansatz integrable spin-1 chain. If we consider the general bilinear-biquadratic $s = 1$ Hamiltonian with

$$H = \sum [\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \beta(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2]$$

then the integrable $\beta = 1$ theory has the $k = 2$ critical theory. There is a gap for $\beta \neq 1$ with a dimerisation transition taking place at the $\beta = 1$ critical point. There is only one relevant operator in the $k = 2$ critical theory permitted by the isotropy and translational symmetries, namely $(\text{Tr } g)^2$, which has $x = 1$, $s_L = s_R = 1$, $s_T = 0$, and hence $2b_i/b = 2$. Thus

$$m \propto |1-\beta|/(\ln|1-\beta|)^2.$$

5. Numerical diagonalisation

The logarithmic corrections make it difficult to extract critical exponents from the diagonalisation of small systems in cases where the Bethe ansatz does not work, in which case L is typically in the range 10-30. However, one way around this problem, which was first exploited by Jullien and Haldane [14], is to study modified Hamiltonians in which the marginal coupling is small. In general, varying any parameter in the microscopic Hamiltonian should vary the marginal coupling constant. Thus we expect to be able to find a point where it vanishes. In the $s = \frac{1}{2}$ model this can be achieved by varying a frustrating second-nearest-neighbour coupling

$$H = \sum_i [\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + J_2(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^2].$$

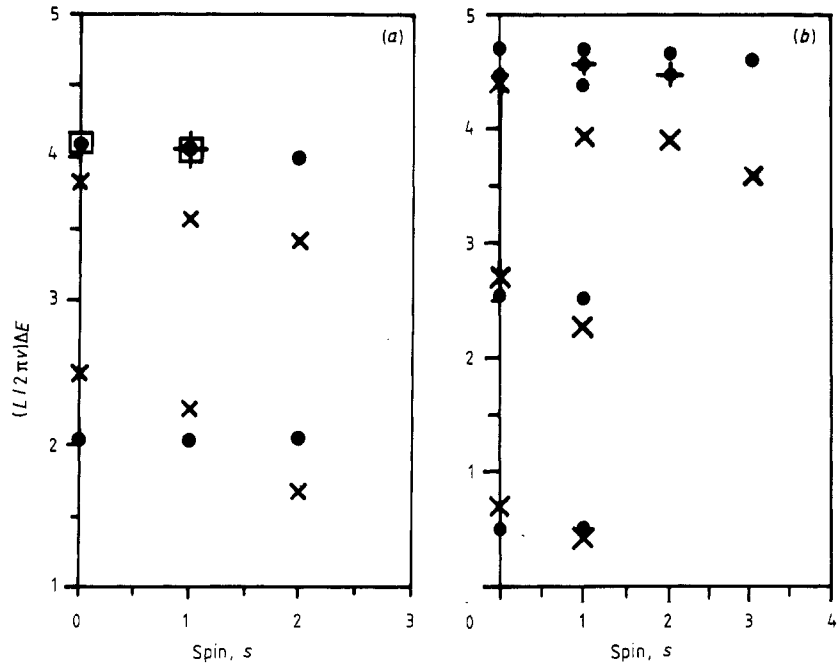


Figure 2. Numerical results for lowest excitation energies of $s=\frac{1}{2}$ chains of length 20, for the model with vanishing log corrections (●, +, □; $J_2/J_1=0.25$), and the pure nearest-neighbour model (×; $J_2=0$), for (*a*) $P=0$ and (*b*) $P=\pi$.

The critical point where g vanishes, separating the gapless and dimerised phases, is [14] at $J_2\approx 0.25$. At this point the ln L corrections are absent and good measurement of the critical exponents can be achieved for $L=20$. The excitation energy of the lowest few states at $P=0$ and π are plotted in figure 2 as a function of their spin. The structure of the conformal towers, with lowest weight $x=0$ and $\frac{1}{2}$ appear very clearly, and these values of x can be measured to a few per cent. The large degeneracy of states at higher energies due to the SU(2)×SU(2) symmetry of the critical theory emerges dramatically. The degeneracies match those given in table 3. The small splittings of the supermultiplets, in this case, is *not* determined by the marginal operator, but by the irrelevant operators, and should be $O(1/L^2)$. For comparison we also show a few of the excitation energies for the pure nearest-neighbour model with the same length, 20. Note that the ln L corrections produce a much larger splitting of the supermultiplets in this case.

6. Bethe ansatz

Recent progress in extending the Bethe ansatz solution to finite-size systems allows checks on the above analytic predictions. These confirm the identification of the critical theory as well as the general principles of conformal field theory.

There are actually two types of finite-size Bethe ansatz results with which we can make comparisons. Analytic expansions for energies in powers of $1/L$, $1/\ln L$, etc

have been calculated from the Bethe ansatz. These measure the universal renormalisation group coefficients, b_i. Also numerical Bethe ansatz results exist for large chains of specified length. These allow measurement of the effective coupling, $g(L)$, at intermediate L before the asymptotic behaviour, $1/\pi b \ln L$ has been reached.

6.1. Analytic results

Woynarovich and Eckle [8] have calculated the excitation energies of a class of states to $O(1/L \ln L)$ and the ground-state energy up to order $1/L(\ln L)^3$ for the integrable $s=\frac{1}{2}$ Heisenberg chain. The states that they consider are those of lowest energy for given s. Such states have the minimum possible s_L, s_R: $s_L = s_R = s/2$, and hence $\boldsymbol{S}_L \cdot \boldsymbol{S}_R = s^2/4$. They are on the envelope of one of the two conformal towers (that with $s_L = s_R = 0$ or $\frac{1}{2}$ for s even or odd respectively). Thus, using (5) and (8), the excitation energies, as a function of s are

$$E_i - E_0 = \tfrac{1}{2}(2\pi v/L)(1-\tfrac{1}{2}\ln L)s^2.$$

This agrees with [8] when $v=\pi/2$, the value determined from the Bethe ansatz at $L=\infty$.

Our analytic formula for the ground-state energy, (9) is

$$E_0/L = \varepsilon_0 - (\pi v/6L)[1+\tfrac{3}{8}(\ln L)^3].$$

Inserting $v=\pi/2$ gives the result of Woynarovich and Eckle except that they have the factor of $\frac{3}{8}$ replaced by 0.3433. We do not understand this discrepancy.

Numerical Bethe ansatz results were obtained for the ground-state energy and the gap to the lowest (triplet) excited state by Woynarovich and Eckle [8] for chains of length up to 1024 for the $s=\frac{1}{2}$ model. We have extended this to $L=2048$ and also calculated the gap to the lowest singlet excited state, which is the other element of the $(\frac{1}{2},\frac{1}{2})$ multiplet at $P=\pi$. We have also calculated the same quantities for the integrable $s=1$ and $s=\frac{3}{2}$ models up to $L=250$ and 100 respectively.

Numerical results for the eigenvalues of the exactly solvable spin-s chains are obtained by finding the complex solutions [6] of

$$[(\lambda_j - \mathrm{i}s)/(\lambda_j + \mathrm{i}s)]^L = -\prod_{k=1}^{l} (\lambda_j - \lambda_k - \mathrm{i})/(\lambda_j - \lambda_k + \mathrm{i}) \qquad j = 1, \ldots, l. \tag{10}$$

The energy and momentum of the state then are given [6] by

$$E = -\sum_{jm=1}^{l} s/(s^2 + \lambda_j^2) \tag{11a}$$

$$P = \sum_{j=1}^{l} [2\tan^{-1}(\lambda_j/s) - \pi] \qquad \mod 2\pi. \tag{11b}$$

In the thermodynamic limit $L \to \infty$, the structure of the ground state and of the low-lying excited states has been discussed by Faddeev and Takhtajan [25], Takhtajan [6], and by Babujian [7]. These authors find that the solutions to (9) are grouped in n-strings of the form:

$$\lambda_{j,\alpha} = \lambda_j + (\mathrm{i}/2)(n+1-2\alpha) \qquad \alpha = 1, \ldots, n$$

where the 'centre' λ_j is real.

For finite L we find deviations from this structure. In particular, the imaginary parts of the solutions are generally *not* interger multiples of i/2. The structure of the solutions for different states, as observed in our numerical calculations, is as follows.

$s=\frac{1}{2}$. In the ground state there are $L/2$ real λ. The lowest triplet excited state with $P-P_0=\pi$ (P_0 is the momentum of the ground state) has $L/2-1$ real λ, whereas the singlet excited state has $L/2-2$ real λ plus a complex pair at *exactly* $\pm i/2$.

$s=1$. In the ground state there are $L/2$ complex pairs, with $|\mathrm{Im}\,\lambda_j|=\frac{1}{2}+\varepsilon_j$, and $\varepsilon_j>0$. In the triplet excited state there are $L/2-1$ such pairs, but now with $\varepsilon_j<0$, plus one λ equal to 0. In the singlet state there are again $L/2-1$ pairs with $\varepsilon_j<0$, plus a pair at *exactly* $\pm i$.

$s=3/2$. In the ground state there are $L/2$ real λ and $L/2$ complex pairs with $|\mathrm{Im}\,\lambda_j|=1+\varepsilon_j$ and $\varepsilon_j>0$. The triplet excited state has $L/2-1$ real λ and $L/2$ complex pairs, now with $\varepsilon_j<0$. The singlet state has $L/2-2$ real λ and $L/2-1$ pairs, again with $\varepsilon_j<0$, plus four λ at $\pm i/2$, $\pm 3i/2$.

In all cases the λ are distributed symmetrically in the complex plane, i.e. if λ is part of the solution, then $-\lambda$ and λ^* also are. The contributions of the complex pairs at $\pm is$ to the energy and momentum of the singlet excited states are obtained from (11) by the limiting process $\lambda=\pm is+\Delta$, $\Delta\to 0$. In this way one obtains $P-P_0=\pi$ for all the singlet excited states discussed here.

The structure of the states considered here for $s=\frac{1}{2}$ agrees with the conclusions of Faddeev and Takhtajan [25]. On the other hand, the structure we find for the singlet excited states for $s=1$ and $\frac{3}{2}$ is apparently quite different from that found by Takhtajan [6], who finds a combination of a '1-string' and a '3-string' ($s=1$) or of a '2-string' and a '4-string' ($s=\frac{3}{2}$). Finally, we remark that in all cases ε_j decreases with increasing L, so that in the limit $L\to\infty$ one recovers the string-type states discussed previously, [6, 7, 25] at least for the ground state. However, at finite L it is extremely important to allow for non-zero ε_j; setting $\varepsilon_j=0$ from the outset, i.e. considering only the centres of the strings, one finds $c=1$ *for all values of* s, an obviously incorrect result (this can actually be shown analytically). On the other hand, the small but non-zero values of ε_j make the numerical solution of (10) quite difficult because some of the factors become extremely rapidly varying. This is why we were unable to go beyond $L=256$ for $s=1$ or $L=100$ for $s=\frac{3}{2}$, whereas for $s=\frac{1}{2}$, where there are no complex pairs, even $L=2048$ could be handled fairly easily.

We use these data to extract three different values of the effective coupling constant at length scale L. These are given by

$$E_0-\varepsilon_0 L=(2\pi v/L)[3k/(2+k)+(2\pi g_c)^3/\sqrt{3}k]$$

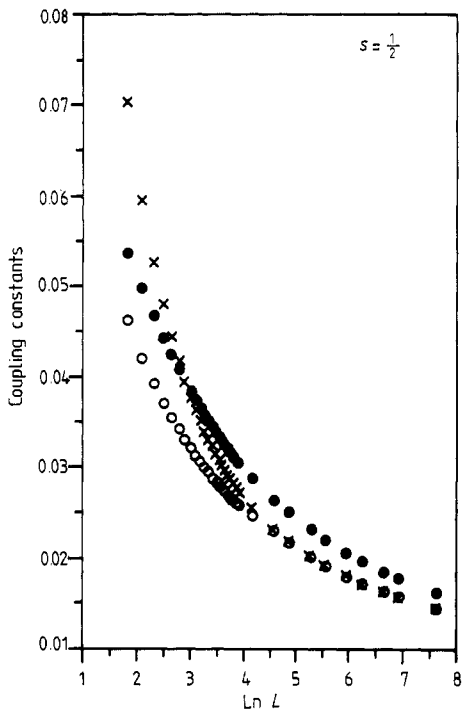
$$E_t-\varepsilon_0 L=(2\pi v/L)[3/2(2+k)-\pi g_t/\sqrt{3}k]$$

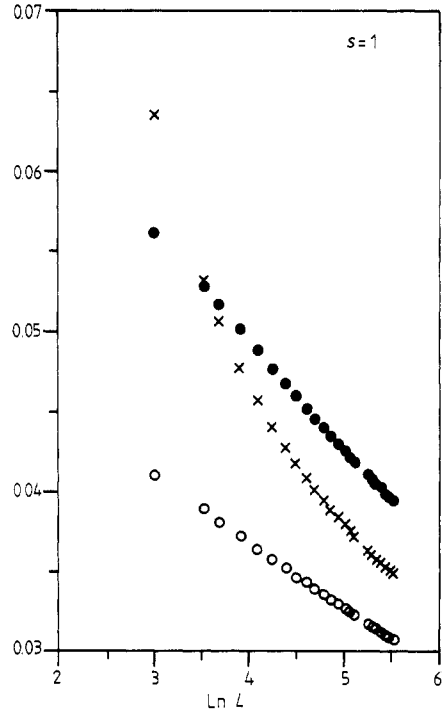
$$E_s-\varepsilon_0 L=(2\pi v/L)[3/2(2+k)+\sqrt{3}\pi g_s/k].$$

Here k is 1, 2 and 3 for the $s=\frac{1}{2}$, 1 and $\frac{3}{2}$ models, respectively. ε_0 is the exact ground-state energy per spin and v is the velocity, both determined from the $L=\infty$ Bethe ansatz. The values of $g_c(L)$, $g_t(L)$ and $g_s(L)$ are plotted against $\ln L$ for the three different models in figure 3. The fact that all three couplings go to zero for large L shows that the $O(1/L)$ predictions are correct. When g is small, the three couplings, g_c, g_s and g_t should approach each other, since they differ by amounts of $O(g^2)$. For values of L at which g is small it should vary with L according to the one-loop β function result

$$g(L)=g(L_0)/[1+4\pi g(L_0)(\ln L/L_0)/\sqrt{3}k].$$

We see that all the couplings do seem to be quite small, even for only moderately large L. This is deceptive, however. The normalisation of g which we have chosen,





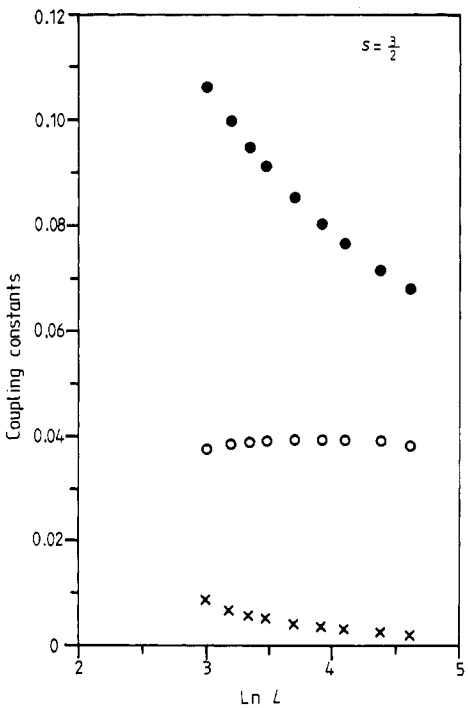


Figure 3. Effective coupling constants, g_t (○), g_s(●) and g_e(×) measured from the triplet excitation energy, singlet excitation energy and ground-state energy, respectively, plotted as functions of length, L, from the Bethe ansatz, for $s = \frac{1}{2}, 1, \frac{3}{2}$.

following Cardy, was determined by normalising the two-point function of the marginal operator. It does not necessarily reflect the true expansion parameter, i.e. the size of the $O(g^2)$ corrections. This is difficult to estimate without doing perturbation theory to $O(g^2)$, but if we simply determine it from the one-loop β function we estimate the true expansion parameter as

$$g_{\text{exp}} \approx 4\pi g/\sqrt{3}k.$$

These estimates could easily be wrong by a factor of 2 or more. Thus the actual expansion parameters are *not* so small for chains of moderate length. In the $s=\frac{1}{2}$ case, g_{exp} ranges from about 0.26 at $L=20$ to 0.11 at $L=2048$, i.e. the coupling is barely small enough that first-order perturbation theory is useful. The three different estimates of g for the largest L differ by about $0.1g$, i.e. $\delta g_{\text{exp}} \approx O(g_{\text{exp}}^2)$ as expected. In the $s=1$ case the range of g_{exp} is from 0.27 at $L=20$ to 0.17 at $L=256$. Again the variation in g_{exp} is $O(g_{\text{exp}}^2)$. For the $s=\frac{3}{2}$ model the average value of g_{exp} is about 0.12 by the above estimate. We suspect that this rather badly underestimates g_{exp} in this case; i.e. the $O(g^2)$ corrections seem to be quite important, given the large variation in the estimates of g.

The flow of the coupling with L (for the average of g_s, g_t and g_c) is compared with the $O(g)$ renormalisation group result of (6), for the $s=\frac{1}{2}$ model, in figure 4. We see that even at the largest available length, 2048, the coupling is barely small enough for the $O(g)$ result to hold.

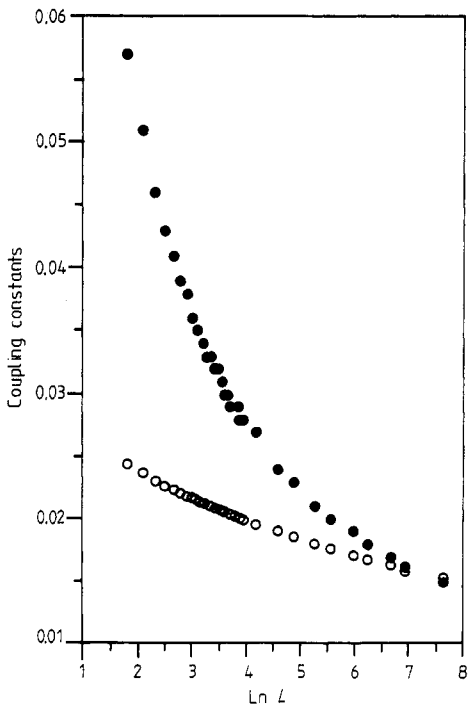


Figure 4. Comparison of the average effective coupling constant $g_{\text{av}} \equiv (g_s + g_t + t_c)/3$ (●) with the one-loop renormalisation group prediction (with a particular choice for g_0) g_{rg} (○), as functions of L for $s=\frac{1}{2}$.

Acknowledgments

We would like to thank F D M Haldane for very useful conversations. The research of IA was partially supported by the Natural Sciences and Engineering Research Council of Canada. That of DG was supported by the National Science Foundation (USA) under grant PHY-80-19754. HJS was granted computing time by Centre de Calcul Vectoriel pour la Recherche, Palaiseau, France. The research of TZ was partially supported by the National Science Foundation (USA) under grant DMR-85-20190 and the New Jersey Supercomputing Fund. He performed computations at the John von Neumann Supercomputer Center and thanks the Aspen Center for Physics for hospitality.

References

[1] Affleck I 1985 *Phys. Rev. Lett.* **55** 1355; 1986 *Nucl. Phys.* B **265** [FS15] 409
[2] Ziman T and Schulz H J 1987 *Phys. Rev. Lett.* **59** 140
[3] Affleck I and Haldane F D M 1987 *Phys. Rev.* B **36** 5291
[4] Haldane F D M 1983 *Phys. Lett.* **93A** 464; 1983 *Phys. Rev. Lett.* **50** 1153; 1985 *J. Appl. Phys.* **57** 3359
[5] Zamolodchikov A B and Fateev V A 1980 *Yad. Fiz.* **32** 587
Kulish P and Sklyanin E 1982 (*Lecture Notes in Physics* **151**) (Berlin: Springer)
Kulish P, Reshetikhin N Yu and Sklyanin E 1981 *Lett. Math. Phys.* **5** 393
[6] Takhtajan L 1982 *Phys. Lett.* **87A** 479
[7] Babudjian J 1982 *Phys. Lett.* **90A** 479; 1983 *Nucl. Phys.* B **215** 317
[8] Woynarovich F and Eckle H-P 1987 *J. Phys. A: Math. Gen.* **20** L443
[9] Cardy J L 1984 *J. Phys. A: Math. Gen.* **17** L385
[10] Cardy J L 1986 *Nucl. Phys.* B **270** 186
[11] Cardy J L 1986 *J. Phys. A: Math. Gen.* **19** L1093
[12] Privman V and Fisher M E 1984 *Phys. Rev.* B **30** 322
[13] Blote H W, Cardy J L and Nightingale M P 1986 *Phys. Rev. Lett.* **56** 742
Affleck I 1986 *Phys. Rev. Lett.* **56** 746
[14] Julien R and Haldane F D M 1983 *Bull. Am. Phys. Soc.* **28** 34
Haldane F D M 1988 *Phys. Rev. Lett.* **60** 635
[15] Affleck I 1987 *Infinite Lie Algebras and Conformal Invariance in Condensed Matter and Particle Physics* ed K Dietz and V Rittenberg (Singapore: World Scientific) p 1
[16] Alcaraz F C, Barber M N and Batchelor M T 1987 *Phys. Rev. Lett.* **58** 771; 1988 *Ann. Phys., NY* **182** 280
[17] Hamer C J, Quispel G R W and Batchelor M T 1987 *J. Phys. A: Math. Gen.* **20** 5677
Hamer C J, Batchelor M T and Barber M N 1988 *J. Stat. Phys.* in press
[18] Alcaraz F C and Martins M J 1988 *J. Phys. A: Math. Gen.* **21** L381; 1989 *J. Phys. A: Math. Gen.* in press
[19] Batchelor M R, Barber M N and Pearce P A 1989 *J. Stat. Phys.* in press
[20] Witten E 1984 *Commun. Math. Phys.* **92** 455
[21] Affleck I 1985 *Phys. Rev. Lett.* **55** 1355
[22] Knizhnik V and Zamolodchikov A B 1984 *Nucl. Phys.* B **247 83**
Zamalodchikov A B and Fateev V A 1986 *Yad. Fiz.* **43** 1031 (*Sov. J. Nucl. Phys.* **43** 657)
Gepner D and Witten E 1986 *Nucl. Phys.* B **278** 493
[23] Affleck I 1986 *Phys. Rev. Lett.* **56** 2763
[24] Kadanoff L P 1981 *Phys. Rev.* B **22** 1405
Nauenberg M and Scalapino D J 1981 *Phys. Rev. Lett.* **22** 837
[25] Faddeev L D and Takhtajan L A 1981 *Phys. Lett.* **85A** 375