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Critical behaviour of mixed Heisenberg chains

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Abstract. The critical behaviour of anisotropic Heisenberg models with two kinds of antiferromagnetically exchange-coupled centres are studied numerically by using finite-size calculations and conformal invariance. These models exhibit the interesting property of ferrimagnetism instead of antiferromagnetism. Most of our results are centred in the mixed Heisenberg chain where we have at even (odd) sites a spin-S (S') SU(2) operator interacting with a XXZ-like interaction (anisotropy Δ). Our results indicate universal properties for all these chains. The whole phase, $1 > \Delta > -1$, where the models change from ferromagnetic ($\Delta = 1$) to ferrimagnetic ($\Delta = -1$) behaviour is critical. Along this phase the critical fluctuations are ruled by a $c = 1$ conformal field theory of Gaussian type. The conformal dimensions and critical exponents, along this phase, are calculated by studying these models with several boundary conditions.

1. Introduction

The critical properties of one-dimensional regular Heisenberg spin chains with one kind of antiferromagnetically exchange-coupled spins have been extensively studied in the literature. The prototype of these models is the anisotropic $S = \frac{1}{2}$ Heisenberg model or XXZ chain [1]. This model is exactly integrable with a critical line of continuously varying critical exponents as we change the anisotropy (Δ), bringing the model from the ferromagnetic ($\Delta = 1$) to the antiferromagnetic ($\Delta = -1$) isotropic points. With the advance of the conformal invariance ideas [2] the whole operator content of this model was obtained [3, 4]. The critical fluctuations are governed by a Gaussian-type conformal field theory with conformal anomaly $c = 1$ and, moreover, the underlying currents satisfying a U(1) Kac–Moody algebra [5].

The extension of the XXZ chain to higher spins $S > \frac{1}{2}$ attracted considerable attention after Haldane [6] conjectured that, for the isotropic antiferromagnetic point ($\Delta = -1$), the model is critical or not depending if S is half-odd-integer or integer, respectively. Consistent with this conjecture, numerical calculations [7–9] indicate that in the case of half-odd-integer spins the models are critical in the whole range of anisotropies ($1 \geqslant \Delta \geqslant -1$) from the ferromagnetic to the antiferromagnetic point. In the case where S is integer, a critical line starting at the ferromagnetic point ends at Δ_c before the antiferromagnetic phase ($\Delta_c > -1$) entering the massive Haldane phase [7–9]. For all spins the massless phases are ruled by a $c = 1$ Gaussian-like conformal field theory [8].

In this paper we extend these studies by studying a quantum chain in which two types of antiferromagnetically exchange-coupled spins S and S' are located at alternate sites.

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When $S \neq S'$, according to a theorem due to Lieb and Mattis [10], the isotropic model ($\Delta = -1$) exhibits ferrimagnetic order, with a $(S - S')\frac{L}{2}$-degenerate ground state, where L is the chain length. Consequently as we vary the anisotropy the model goes from the ferromagnetic point ($\Delta = 1$) to the ferrimagnetic point ($\Delta = -1$). We studied these models for $(S, S') = (\frac{1}{2}, 1)$ and $(S, S') = (\frac{1}{2}, \frac{3}{2})$, using finite-size scaling and conformal invariance [2]. To supplement our studies we considered two other anisotropic models that also exhibit ferrimagnetic behaviour at the isotropic point. Our studies show that all these models between the two (ferromagnetic and ferrimagnetic) isotropic points $1 > \Delta > -1$ have a universal Gaussian critical behaviour with central charge $c = 1$. In this massless phase the critical exponents exhibit a model-dependent variation with the anisotropy.

The paper is organized as follows. In section 2 we define the (S, S')-Heisenberg chain and review some results obtained from conformal invariance in the model with $S = S'$. In sections 3 and 4 we present our numerical results for the (S, S')-Heisenberg model and related models. Finally in section 5 we present our general conclusions.

2. The model and conformal invariance relations

The mixed Heisenberg quantum chains are defined by attaching an SU(2) spin-S at the odd sites ($\boldsymbol{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$; $i = 1, 3, 5, \ldots$) and a spin S' at the even sites ($\boldsymbol{S}_i = (S_i^x, S_i^y, S_i^z)$; $i = 2, 4, 6, \ldots$). The Hamiltonian on an L (even) site chain, with periodic ends, is defined by

$$H = -\sum_{i=1}^{L/2} (\sigma_{2i-1}^x S_{2i}^x + \sigma_{2i-1}^y S_{2i}^y + \Delta \sigma_{2i-1}^z S_{2i}^z) \tag{1}$$

where Δ is the anisotropy constant. This Hamiltonian, like the standard spin-S XXZ chain ($S = S'$), has a U(1) symmetry due to its commutation with the z component of the total spin

$$S_z = \sum_{i=1}^{L/2} (\sigma_{2i-1}^z + S_{2i}^z). \tag{2}$$

For $\Delta > 1$ the model is massive and ferromagnetic with a double degenerate ground state corresponding to the two fully ordered states with $S_z = \pm\frac{L}{2}(S + S')$. At $\Delta = 1$ the lowest energy in all U(1) sectors

$$\left(S_z = -\frac{L}{2}(S + S'), -\frac{L}{2}(S + S') + 1, \ldots, \frac{L}{2}(S + S') - 1, \frac{L}{2}(S + S') \right)$$

are degenerate, rendering a ferromagnet ground state with total spin $\frac{L}{2}(S+S')$ and a massless spectra with a quadratic dispersion relation. For $1 > \Delta > -1$ the ground state is single or double degenerate, depending on if $|S-S'|\frac{L}{2}$ is integer or half-odd-integer and belongs to the sectors with $S_z = 0$ or $S_z = \pm\frac{1}{2}$, respectively. At $\Delta = -1$ the lowest energies in the sectors where $S_z = -\frac{L}{2}|S - S'|, -\frac{L}{2}|S - S'| + 1, \ldots, \frac{L}{2}|S - S'| - 1, \frac{L}{2}|S - S'|$ become degenerate and we have ferrimagnetic order [10]. For $\Delta < -1$ the ground state is double degenerate, occurring in the sectors with $S_z = \pm\frac{L}{2}|S - S'|$, and we expect a massive behaviour as in the standard $S = S'$ XXZ chain. In order to illustrate the spectral dependence on the anisotropy Δ, in figure 1 we draw, in schematic form, the location of the lowest eigenenergies of (1) in the various S_z sectors.

Our analysis indicates that in the whole region $1 \geqslant \Delta \geqslant -1$ the model is critical, like the $S = \frac{1}{2}$ XXZ model ($S = S' = \frac{1}{2}$). We assume that the Hamiltonian (1), like most

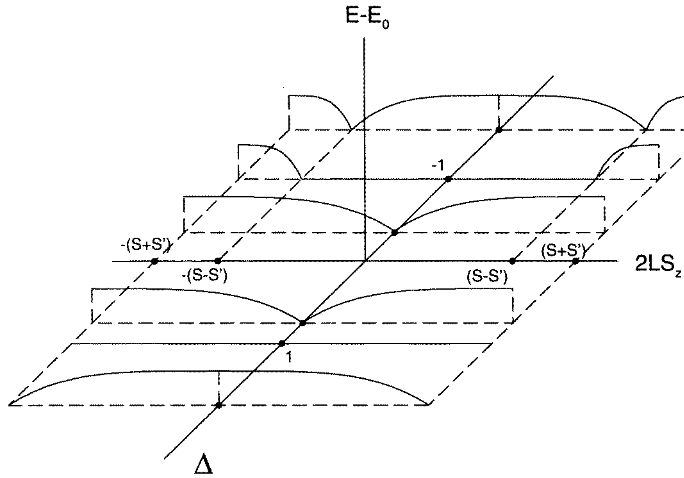

Figure 1. Schematic values of the lowest eigenenergy in a sector with magnetization S_z of the Hamiltonian (1). The ground-state energy is E_0 and $(S - S')\frac{L}{2}$ is an integer.

statistical mechanics quantum chains are conformally invariant in its critical regime. Under this assumption the machinery arising from conformal invariance tells us that, for each primary operator [2, 11] O_α with dimension x_α and spin s_α in the Virasoro operator algebra of the infinite system, there exists an infinite tower of states, in the quantum Hamiltonian, for a periodic chain of L sites, whose energy and momentum as $L \to \infty$ are given by

$$E^{\alpha}_{j,j'} = E_0(L) + \frac{2\pi}{L} v(x_\alpha + j + j') + \mathrm{o}(L^{-1}) \tag{3}$$

and

$$P^{\alpha}_{j,j'} = \frac{2\pi}{L}(s_\alpha + j - j') \tag{4}$$

where $j, j' = 0, 1, \ldots$. Here $E_0(L)$ is the ground-state energy and v is the velocity of sound, which can be determined by the energy-momentum dispersion relation or from the difference among consecutive energy levels in a same conformal tower. The finite-size corrections of the ground-state energy also give a way to calculate the conformal anomaly. For periodic chains, the ground-state energy behaves asymptotically as [12]

$$\frac{E_0(L)}{L} = e_\infty - \frac{\pi c v}{6L^2} + \mathrm{o}(L^{-2}) \tag{5}$$

where e_∞ is the ground-state energy per site in the bulk limit.

In the case where $S = S'$ a critical phase appears [7–9] in (1) for anisotropies $1 \geqslant \Delta \geqslant \Delta_c(S)$, where due to the Haldane conjecture [6], $\Delta_c = -1$ or $\Delta_c > -1$ depending if S is half-odd-integer or not. This massless phase is described by a U(1) conformal field theory with central charge $c = 1$ [8]. The anomalous dimensions, x_α, appearing through (3) in the U(1) sector $S_z = n$ of the Hamiltonian (1) with periodic ends are given by

$$x_{n,m} = n^2 x_p + \frac{m^2}{4x_p} \qquad n, m = 0, \pm 1, \pm 2, \ldots \tag{6}$$

where x_p depend on S and Δ. For $S = S' = \frac{1}{2}$ we have the exact dependence [3, 4] $x_p = (\pi - \cos^{-1}(-\Delta))/2\pi$. Although the model is not integrable for $S = S' > \frac{1}{2}$, numerical calculations indicate the conjecture [8]

$$x_p = (\pi - \cos^{-1}(-\Delta))/4\pi S \qquad \text{for } -1 < \Delta \lesssim 0.$$

Beyond the dimensions (6) other integer dimensions also appear in the sector with $S_z = n = 0$. This fact indicates that the underlying conformal field theory satisfies a larger algebra than the Virasoso conformal algebra, namely, a U(1) Kac–Moody algebra [5, 8]. The dimensions (6) correspond to operators $O_{n,m}$ and the number of its descendants will be given by the product of two U(1) Kac–Moody characters. The dimensions (6) indicate that the operators $O_{n,m}$ correspond to the Gaussian model operators [13] composed of a spin-wave excitation of index, n, and a 'vortex' excitation of vorticity, m.

Other interesting properties of these $c = 1$ critical phases appear when we consider these chains with more general boundary conditions, compatible with its U(1) symmetry, i.e. by preserving the total spin, S_z, as a good quantum number. Two of these conditions are, the $x - y$ twisted boundary conditions

$$S^x_{L+1} \pm \mathrm{i}S^y_{L+1} = \mathrm{e}^{\pm\mathrm{i}\Phi}(S^x_1 \pm \mathrm{i}S^y_1) \tag{7}$$

$$S^z_{L+1} = S^z_1 \tag{8}$$

where Φ is an arbitrary angle, and free boundary conditions

$$S^x_{L+1} = S^y_{L+1} = S^z_{L+1} = 0. \tag{9}$$

The net effect of the boundary angle, Φ, in the dimensions (6) is to shift the spin-wave index by an amount [3, 8] $\Phi/2\pi$,

$$x_{n,m+\Phi/2\pi} = n^2 x_p + \frac{(m + \Phi/2\pi)^2}{4x_p}. \tag{10}$$

In a semi-infinite lattice the correlation functions involving lattice points near the surface have a power-law decay distinct from the case where the points are away from the surface (bulk behaviour). These correlations are ruled by the surface exponents x_s. These exponents can be obtained from the finite-size corrections of the mass-gap amplitudes of finite chains with free ends. Instead of (3) and (4), to each surface exponent of the semi-infinite system, at the critical point, there exists a set of states with energies given by [11]

$$E^{(F)}_r = E^{(F)}_0(L) + \frac{\pi v}{L}(x_s + r) + \mathrm{o}(L^{-1}) \tag{11}$$

where $E^{(F)}_0(L)$ is the ground-state energy of the L-site chain and $r = 0, 1, 2, \ldots$. Instead of (5) we have [12]

$$\frac{E^{(F)}_0(L)}{L} = e_\infty + \frac{f_\infty}{L} - \frac{\pi c v}{24L^2} + \mathrm{o}(L^{-2}) \tag{12}$$

where f_∞ is the bulk limit of the surface energy. The study of (1) with $S = S'$ and free ends [8, 14] shows that, in the critical region, for each sector $S_z = n$ there appears only one conformal tower associated to the dimensions

$$x_s(n) = 2n^2 x_p \qquad n = 0, 1, 2, \ldots \tag{13}$$

with the multiplicity of its descendants given by the character of a single U(1) Kac–Moody algebra [8, 15].

Table 1. Estimates for some values of the anisotropy, Δ, of the conformal anomaly of the (S, S')-Heisenberg chain (1) for $(S, S') = (\frac{1}{2}, 1)$ and $(S, S') = (\frac{1}{2}, \frac{3}{2})$.

(S, S')	$\Delta = .8090$	$\Delta = 0.5$	$\Delta = 0$	$\Delta = -0.5$	$\Delta = -0.7071$
$(\frac{1}{2}, 1)$	0.93 ± 0.05	1.01 ± 0.01	1.03 ± 0.04	1.01 ± 0.01	0.9 ± 0.1
$(\frac{1}{2}, \frac{3}{2})$	1.00 ± 0.01	0.99 ± 0.01	1.000 ± 0.005	1.00 ± 0.01	0.9 ± 0.1

3. Results for the mixed Heisenberg chains

We calculate numerically the eigenspectra of the Hamiltonian (1) by using the Lanczos method in the cases where $(S, S') = (\frac{1}{2}, 1)$ and $(S, S') = (\frac{1}{2}, \frac{3}{2})$ up to lattice sizes $L = 20$ and $L = 16$, respectively. Our results, for several boundary conditions, indicate that in the whole region, $1 \geqslant \Delta \geqslant -1$, the model is gapless and conformally invariant. The ground state in this region will have the lowest possible value of $|S_z|$. It is non-degenerate with $S_z = 0$ if $\frac{L}{2}|S - S'|$ is integer and is doubled degenerate with $S_z = \pm\frac{1}{2}$, otherwise. Consequently in order to obtain a uniform convergence of our finite-size results we consider in the case $(S, S') = (\frac{1}{2}, 1)$ only lattice sizes which are multiples of 4.

Let us consider initially the case of periodic chains. The model is invariant under translation by a unit cell with two spins, with momentum $p = \frac{4\pi}{L} l (l = 0, 1, \ldots, \frac{L}{2} - 1)$. In order to calculate the conformal anomaly and exponents from equations (3)–(5) we should estimate the sound velocity. As in the $S = S' = \frac{1}{2}$ case the lowest eigenenergy with non-zero momentum (modulo π) belonging to the ground-state sector is associated to a primary spin-1 operator with dimension equal to unity for all values of Δ. Using equation (3) we obtain an estimate for the sound velocity

$$v(L) = \frac{\left(E_{4\pi/L} - E_0(L)\right) L}{2\pi} \tag{14}$$

where $E_0(L)$ is the ground-state energy and $E_{4\pi/L}$ is the lowest eigenenergy of a state with momentum $4\pi/L (\mathrm{mod}\, \pi)$. Using (14) the conformal anomaly c is obtained by extrapolating the numerical sequence obtained from (5). In table 1 we show, for some values of Δ, our estimates for c in the two cases $(S, S') = (\frac{1}{2}, 1)$ and $(S, S') = (\frac{1}{2}, \frac{3}{2})$. All the extrapolated results reported in this table, as in the subsequent ones, are calculated by using the alternating ϵ-algorithm [16], which is a variant of the van den Broeck–Schwartz method [17]. The errors are roughly estimated from the region of stability of these approximants. It was not possible to obtain reliable results near the isotropic points $\Delta = 1$ and $\Delta = -1$. This happens because, as near the ferromagnetic models with $S = S'$ [8], the sound velocity decreases towards zero as we tend towards the isotropic point (the energy-momentum dispersion relation changes from linear to quadratic). Our results indicate that we have a conformal anomaly $c = 1$ in both cases and we believe that this is the general case for arbitrary $S \neq S'$, since the spectrum (see figure 1) shows the same essential features independently of S and S' being integer or half-odd-integer. Moreover the vanishing of the sound velocity as we tend toward the ferromagnetic ($\Delta = 1$) and ferrimagnetic ($\Delta = -1$) points indicate that the critical fluctuations around the ferrimagnetic point are similar to those near the ferromagnetic point. As we see in table 1 the results for $(S, S') = (\frac{1}{2}, \frac{3}{2})$ are slightly better than those of $(S, S') = (\frac{1}{2}, 1)$. This is due to the fact that for $(S, S') = (\frac{1}{2}, \frac{3}{2})$ the number of terms in the finite-size sequences are larger since L can be an arbitrary even number.

The conformal dimensions are calculated by using (3) and (14). For example in the (S, S') chain the lowest energy, E_n, in the sector with total spin, $S_z = n$, is associated

Table 2. Extrapolated values of the finite-size sequences (15) for the Hamiltonian (1) with $(S, S') = (\frac{1}{2}, 1)$ and some values of the anisotropy Δ. The extrapolations in the third and fourth column are obtained from the sequences $x_2^{1/2,1}(L)/x_1^{1/2,1}(L)$ and $x_1^{1/2,1}(L)/x_1^{1/2,1/2}(L)$, respectively. The values of $x_1^{1/2,1}$ in the fifth column are obtained from standard finite-size scaling (see equation (18)).

Δ	$x_1^{\frac{1}{2},1}$	$x_2^{\frac{1}{2},1}$	$x_2^{\frac{1}{2},1}/x_1^{\frac{1}{2},1}$	$x_1^{\frac{1}{2},1}/x_1^{\frac{1}{2},\frac{1}{2}}$	$1-\gamma_p/2\nu$
0.917 2	0.0414 ± 0.0001	0.165 ± 0.001	3.9996 ± 0.0005	0.664 ± 0.005	0.038
0.809 01	0.0639 ± 0.0005	0.255 ± 0.001	3.9999 ± 0.0005	0.653 ± 0.008	0.069
0.5	0.1041 ± 0.002	0.415 ± 0.001	3.999 ± 0.005	0.626 ± 0.001	0.104
0.173 6	0.1302 ± 0.0005	0.521 ± 0.004	3.99 ± 0.01	0.584 ± 0.002	0.129
0	0.139 ± 0.001	0.554 ± 0.002	3.999 ± 0.004	0.554 ± 0.002	0.138
−0.5	0.136 ± 0.001	0.547 ± 0.005	4.01 ± 0.01	0.40 ± 0.01	0.134
−0.707 1	0.105 ± 0.005	0.44 ± 0.02	4.01 ± 0.01	0.31 ± 0.01	0.111
−0.901 0	0.035 ± 0.005	0.15 ± 0.02	3.99 ± 0.02	0.11 ± 0.01	0.066

with the dimension $x_n^{S,S'}$, which is calculated from the asymptotic $(L \to \infty)$ value of the sequence

$$x_n^{S,S'}(L) = \frac{E_n(L) - E_0(L)}{2\pi v(L)} \tag{15}$$

where $v(L)$ is given by (14). In tables 2 and 3 we show our results for $n = 1$, 2 and some values of the anisotropy. We see from these tables that for all values of the anisotropy, the extended relation

$$x_n^{S,S'} = n^2 x_1^{S,S'} \tag{16}$$

holds. These dimensions are similar to the Gaussian dimensions, $x_{n,0}$, appearing in (6), on identifying $x_p = x_1^{S,S'}$. Different from the critical regime in the homogeneous spin case $S = S'$, when $S \neq S'$ the dimensions, $x_1^{S,S'}$, increase as we depart from the ferromagnetic point, but around $\Delta \lesssim -0.5$ it starts to decrease again and we have small values of x_p near the ferrimagnetic point, as we normally see near the ferromagnetic point. The small values of the exponents, $x_1^{S,S'}$, near the ferromagnetic and ferrimagnetic points is the signature of the long-range ordered ground state at the isotropic points. The fourth column of these tables also shows that near the ferromagnetic point $x_1^{S,S'} = x_1^{1/2,1/2}/(S+S')$, which give us

$$x_1^{S,S'} = \frac{\pi - \cos(-\Delta)}{2\pi(S+S')} \qquad \Delta \to 1. \tag{17}$$

This result, when compared with the conjectured [8] results for $S = S'$, indicate that near the ferromagnetic point we have essentially a Heisenberg model with effective spin $(S+S')/2$. On the other hand the degeneracy of the ground state at the ferrimagnetic point $(\Delta = -1)$ induce us to expect near this point an effective Heisenberg ferromagnetic chain with effective spin $(S-S')/2$. However, we are not able to make a conjecture as in equation (17).

We also made an independent calculation of the exponents $x_1^{1/2,1}$ by using standard finite-size scaling [18]. This exponent is related to the ratio of the 'electric' susceptibility γ_p [19] and correlation-length exponent ν, by the relation

$$\frac{\gamma_p}{\nu} = 2(1 - x_1^{1/2,1}). \tag{18}$$

Table 3. Extrapolated values of the finite-size sequences (15) for the Hamiltonian (1) with $(S, S') = (\frac{1}{2}, \frac{3}{2})$ and some values of the anisotropy Δ. The extrapolations in the third and fourth column are obtained from the sequences $x_2^{1/2,3/2}(L)/x_1^{1/2,3/2}(L)$ and $x_1^{1/2,3/2}(L)/x_1^{1/2,1/2}(L)$, respectively.

Δ	$x_1^{\frac{1}{2},\frac{3}{2}}$	$x_2^{\frac{1}{2},\frac{3}{2}}$	$x_2^{\frac{1}{2},\frac{3}{2}}/x_1^{\frac{1}{2},\frac{3}{2}}$	$x_1^{\frac{1}{2},\frac{3}{2}}/x_1^{\frac{1}{2},\frac{1}{2}}$
0.9172	0.0310 ± 0.0005	0.124 ± 0.002	3.9995 ± 0.0005	0.50 ± 0.02
0.80901	0.047 ± 0.001	0.189 ± 0.002	4.001 ± 0.001	0.47 ± 0.02
0.5	0.076 ± 0.002	0.301 ± 0.002	4.0000 ± 0.0001	0.44 ± 0.01
0.1736	0.0914 ± 0.0001	0.3661 ± 0.0002	4.0001 ± 0.0001	0.412 ± 0.001
0	0.0959 ± 0.0001	0.384 ± 0.001	4.0000 ± 0.0001	0.383 ± 0.001
−0.5	0.089 ± 0.002	0.357 ± 0.003	4.00 ± 0.04	0.26 ± 0.01
−0.7071	0.071 ± 0.002	0.28 ± 0.01	3.98 ± 0.01	0.19 ± 0.01
−0.9010	0.031 ± 0.001	0.11 ± 0.01	3.99 ± 0.02	0.065 ± 0.008

The ‘electric’ susceptibility is the response of the system to a staggered transversal field. This susceptibility, χ_L^ξ, is calculated by adding an ‘electric field’ interaction $\xi \sum_i (g_A \sigma_i^x + g_B S_{i+1}^x)$ in (1)

$$\chi_L^\xi = \left. \frac{\partial^2 E_0(\xi)}{\partial \xi^2} \right|_{\xi=0} \tag{19}$$

where $E_0(\xi)$ is the ground-state energy in the presence of the ‘electric’ field. The Landé factors g_A and g_B produces the staggering effect of the transverse ‘electric’ field. In the isotropic case $S = S'$ we must choose $g_A/g_B \neq 1$, otherwise it will produce the effect of a uniform transverse field, which is not related with the exponent γ_p. In the case $S \neq S'$ our results show that a similar effect also occurs and in order to calculate γ_p we should consider $g_A/g_B \neq r_c$. For $S = \frac{1}{2}$ and $S' = 1$, r_c changes from $r_c = 2$ to $r_c = 2.66$ as the anisotropy changes from the ferromagnetic point ($\Delta = 1$) to the ferrimagnetic one ($\Delta = -1$). These points are probably related to the compensation mechanism which usually happens in ferrimagnetic ordered models when temperature effects are taken into account [20]. In the bulk limit, $\chi_L^\xi \sim L^{\gamma_p/\nu}$, the extrapolation of the finite-size sequence obtained by choosing $g_A = 0$ and $g_B = 1$ gives from (18) the results in the last column of table 2. In this case, since we calculate lattices up to $L = 16$, it is difficult to obtain an error estimate through the alternating ϵ-algorithm [16]. The results presented are in reasonable agreement with those derived by using the conformal invariance relations. Beyond the dimensions presented in tables 2 and 3 our results also indicate other dimensions which would correspond to $x_{n,m}$ in (6) with $m \neq 0$. Instead of presenting these dimensions we show in table 4 the lowest dimensions $x_\Phi^{S,S'}$ obtained by calculating the (S, S') model with the twisted boundary conditions given by (7) and (8). These dimensions are obtained from the bulk limit extrapolations of the sequence

$$x_\Phi^{S,S'}(L) = \frac{E_\Phi(L) - E_0(L)}{2\pi v(L)} \tag{20}$$

where $E_\Phi(L)$ is the ground-state energy of the Hamiltonian (1) with L sites and boundary conditions (7) and (8). The results given in table 4 indicate that

$$x_\Phi^{S,S'} = \frac{(\Phi/2\pi)^2}{4x_1^{S,S'}} \tag{21}$$

Table 4. Dimensions $x_1^{S,S'}(\Phi)$ obtained from the bulk limit of the finite-sequences (20) obtained from the Hamiltonian (1) with twisted boundary conditions (7) and (8) specified by the angles $\Phi = \pi$ and $\Phi = \frac{4\pi}{3}$. The values in parentheses are the predicted ones obtained by using the values of $x_1^{S,S'}$ estimated in tables 2 and 3 in (21).

	$\Delta = 0.8090$	$\Delta = 0.1736$	$\Delta = 0$	$\Delta = -0.5$	$\Delta = -0.7071$
$x_1^{\frac{1}{2},1}(\Phi = \pi)$	0.93 ± 0.02 (0.978)	0.49 ± 0.01 (0.480)	0.46 ± 0.01 (0.4500	0.48 ± 0.01 (0.460)	0.58 ± 0.01 (0.595)
$x_1^{\frac{1}{2},1}(\Phi = 4\pi/3)$	1.65 ± 0.05 (1.74)	0.86 ± 0.01 (0.853)	0.81 ± 0.01 (0.799)	0.84 ± 0.02 (0.817)	1.03 ± 0.02 (1.06)
$x_1^{\frac{1}{2},\frac{3}{2}}(\Phi = \pi)$	1.26 ± 0.05 (1.33)	0.686 ± 0.002 (0.684)	0.657 ± 0.005 (0.652)	0.70 ± 0.01 (0.702)	0.90 ± 0.03 (0.880)
$x_1^{\frac{1}{2},\frac{3}{2}}(\Phi = 4\pi/3)$	2.22 ± 0.05 (2.36)	1.222 ± 0.004 (1.216)	1.165 ± 0.005 (1.159)	1.25 ± 0.01 (1.248)	1.53 ± 0.04 (1.565)

where $x_1^{S,S'}$ is given in tables 2 and 3. These dimensions correspond to the dimensions $x_{0,\Phi/2\pi}$ in (10). The results presented in tables 2–4 clearly indicate that, in the whole disordered regime, $-1 < \Delta < 1$, the conformal dimensions are those of a Gaussian model. The dimensions are given by (6) where $x_p = x_1^{S,S'}$ is a continuous function of Δ with some of its values given in tables 2 and 3. We have also studied the $(S, S') = (\frac{1}{2}, 1)$ model with lattice sizes $L = 4l + 2$ $(l = 1 - 4)$. In this case the ground state is degenerate as in the standard $S = S' = \frac{1}{2}$ XXZ chain with an odd number of sites [2] and we obtain the dimensions $x_{n+1/2,m}(n, m = 0, \pm 1, \pm 2, \ldots)$.

For completeness, we also calculated the surface exponents of these chains. These exponents are calculated from the eigenspectra of (1) with free boundary conditions. From (11) the surface exponents, $x_s^{S,S'}(n)$, associated with the state with lowest energy, $E_{n,0}^{(F)}$, in the sector $S_z = n$ of the (S, S') chain can be estimated from the large-L behaviour of the sequence

$$F^{S,S'}(n, L) = \frac{E_{n,0}^{(F)} - E_{0,0}^{(F)}}{E_{0,1}^{(F)} - E_{0,0}^{(F)}} \tag{22}$$

where $E_{n,m}^{(F)}$ is the m excited state in the sector $S_z = n$. The estimator (22) was obtained by assuming that as in the $S = S'$ case, the first mass gap amplitude in the ground-state sector is associated with a dimension equal to unity. Our results are shown in table 5 where we clearly see the same type of extended relation as in (16), namely

$$x_s^{S,S'}(n) = n^2 x_s^{S,S'}(1). \tag{23}$$

Comparing these results with those of tables 2 and 3 we obtain the relations (13) expected in a Gaussian model

$$x_s^{S,S'}(n) = 2n^2 x_1^{S,S'} \qquad n = 0, 1, 2, \ldots \tag{24}$$

where $x_1^{S,S'}$ is the dimension which appeared in the periodic case.

4. Results for other related models of ferrimagnetism

Inspired by the results of the last section we will try to see if the general critical features of the (S, S')-Heisenberg models can also be observed in other models exhibiting

Table 5. Surface critical exponents $x_s^{S,S'}(n)$ associated to the lowest eigenergies in the sectors $n = 1, 2$ of the Hamiltonian (1) with $(S, S') = (\frac{1}{2}, 1)$ and $(S, S') = (\frac{1}{2}, \frac{3}{2})$ for some values of Δ. These estimates are obtained from the sequences (22).

Δ	$x_1^{\frac{1}{2},1}$	$x_2^{\frac{1}{2},1}$	$x_1^{\frac{1}{2},\frac{3}{2}}$	$x_2^{\frac{1}{2},\frac{3}{2}}$
0.917 2	0.082 ± 0.002	0.330 ± 0.005	0.061 ± 0.001	0.245 ± 0.005
0.809 01	0.128 ± 0.001	0.513 ± 0.003	0.098 ± 0.003	0.392 ± 0.005
0.173 6	0.258 ± 0.002	1.036 ± 0.003	0.183 ± 0.001	0.73 ± 0.01
0	0.272 ± 0.005	1.106 ± 0.003	0.191 ± 0.001	0.766 ± 0.005
−0.5	0.266 ± 0.002	1.070 ± 0.005	0.181 ± 0.002	0.728 ± 0.005
−0.901 0	0.1086 ± 0.0005	0.440 ± 0.002	0.065 ± 0.005	0.260 ± 0.002

ferrimagnetism. In this direction we will study two other models defined on a bipartite lattice as in figures 2(a) and (b). At each lattice point we attach a spin-$\frac{1}{2}$ operator which interacts along the lines of figure 2 with interactions of XXZ type

$$H = -\sum_{\langle ik\rangle}^{L}(\sigma_i^x\sigma_k^x + \sigma_i^y\sigma_k^y + \Delta\sigma_i^z\sigma_k^z). \tag{25}$$

The first model, defined in the bipartite lattice of figure 2(a), we denote ABC and the second one, in figure 2(b), we denote AB_2. The lattice size L is considered as twice the number of lattice sites in the sublattice A (in figures 2(a) and (b) $L = 6$). Both models, at the isotropic ferromagnetic point, $\Delta = 1$, are fully ordered. At $\Delta = -1$ they show a ferrimagnetic behaviour since the total number of spin variables in each sublattice is not equal. As before the Hamiltonian has a U(1) symmetry and its Hilbert space is separated in the σ^z-basis into block disjoint sectors labelled by the z-component of the total spin $S_z = \sum_i \sigma_i^z$. The ground-state location in these sectors as well as its degeneracies on a finite lattice for $-1 \leqslant \Delta \leqslant 1$ are exactly like those shown in figure 1, on taking $S = \frac{1}{2}$ and $S' = 1$.

Our numerical results for periodic boundary conditions indicate that both models are disordered and massless in the whole regime $1 \geqslant \Delta \geqslant -1$. The thermal effects of the model AB_2 at $\Delta = -1$ are considered in [21]. We now report our results separately for both models.

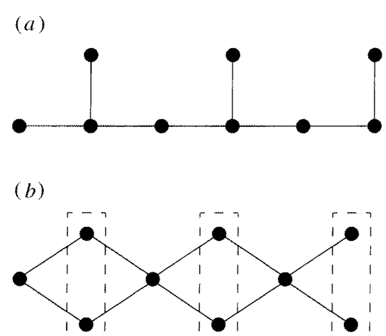

Figure 2. Lattices where (a) the ABC and (b) the AB_2 quantum chains are defined. At the circles we have spin-$\frac{1}{2}$ SU(2) operators and along the lines the interactions are given by (25) (XXZ type). The Hamiltonian AB_2 is invariant under a local gauge transformation which independently interchanges the spin operators inside a rectangle in (b).

Table 6. Anomalous dimensions, x_n^{ABC}, associated to the lowest eigenenergies in the sector $n = 1, 2$ of the model ABC, defined in figure 2(b), for some values of the anisotropy Δ. The third and fourth column are calculated similarly as for tables 2 and 3.

Δ	x_1^{ABC}	x_2^{ABC}	x_2^{ABC}/x_1^{ABC}	$x_1^{ABC}/x_1^{\frac{1}{2},\frac{1}{2}}$
0.917 2	0.07 ± 0.01	0.27 ± 0.02	3.99 ± 0.02	0.86 ± 0.03
0.809 01	0.077 ± 0.003	0.31 ± 0.01	4.01 ± 0.01	0.84 ± 0.02
0.5	0.129 ± 0.002	0.51 ± 0.01	4.00 ± 0.03	0.78 ± 0.02
0.173 6	0.158 ± 0.003	0.635 ± 0.005	4.01 ± 0.02	0.71 ± 0.01
0	0.165 ± 0.002	0.667 ± 0.005	4.01 ± 0.02	0.66 ± 0.01
−0.5	0.152 ± 0.002	0.61 ± 0.01	3.99 ± 0.02	0.45 ± 0.01
−0.707 1	0.121 ± 0.002	0.486 ± 0.002	4.00 ± 0.02	0.32 ± 0.01
−0.901 0	0.05 ± 0.01	0.20 ± 0.01	3.99 ± 0.03	0.11 ± 0.01

4.1. Model ABC

Using equation (14) we observe, as in section 3, that the sound velocity approaches zero as we tend towards the isotropic points $\Delta = \pm 1$. The conformal dimensions, $x_n^{ABC}(n = 1, 2, \ldots)$, associated to the lowest eigenenergy in the sector $S_z = n$ are obtained by extrapolating the sequence (15) for L up to 16. Our results for some dimensions and anisotropies are shown in table 6. As we see in this table, as in (16) the relation $x_n^{ABC} = n^2 x_1^{ABC}$ also holds for the whole range of anisotropies $1 \geqslant \Delta \geqslant -1$, with x_1^{ABC} depending continuously on Δ. Since at $\Delta = 1$ we have the same ground-state degeneracy as in the $(S, S') = (\frac{1}{2}, 1)$ Heisenberg model we would expect an asymptotic behaviour, as $\Delta \to 1$, like (17) with $S = \frac{1}{2}$ and $S' = 1$. However, the fourth column of table 6 tell us this is not true. We have also studied this model with the twisted boundary conditions (7) and (8) with results as predicted in (10), which clearly indicate an underlying $c = 1$ Gaussian-field theory in the whole regime $1 \geqslant \Delta \geqslant -1$.

4.2. Model AB_2

In this case, beyond the U(1) symmetry, we also have a Z(2) local gauge invariance corresponding to an independent interchange of the spin variables located at points like those shown in broken-lined rectangles in figure 2(b). Since we have $L/2$ disjoint sectors labelled by the eigenvalues g_l (± 1) of the gauge operators

$$G_l = \boldsymbol{\sigma}_i . \boldsymbol{\sigma}_k + \tfrac{1}{4} \qquad l = 1, 2, \ldots, L/2 \tag{26}$$

where $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_k$ are the spin-$\frac{1}{2}$ operators located at the lth rectangle, a sector having $g_l = 1$ will be spanned in a basis with three even combinations of the spin variables $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_k$ located at the rectangle l. This means that in σ^z-basis we should have the triplet combination $|++\rangle$, $\frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)$ and $|--\rangle$. On the other hand if $g_l = -1$ we should have a singlet combination $\frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$. It is not difficult to verify that the interaction between spins in the sublattice A with a given neighbouring retangle l with $g_l = 1$ (triplet) is exactly the same as in the $(S, S') = (\frac{1}{2}, 1)$ Heisenberg interaction (see (1)). In contrast, the interaction with a rectangle with $g_l = -1$ (singlet) is zero. This implies some interesting consequences. For a given U(1) sector $S_z = n$ the eigenenergies of the gauge sector with $g_l = 1$ for all $l = 1, 2, \ldots, L/2$ of the Hamiltonian AB_2 with periodic ends will be exactly the same as the $S_z = n$ sector of the $(S, S') = (\frac{1}{2}, 1)$ Heisenberg chain (1), also with a periodic boundary condition. For general gauge choices we lose translation invariance since the operator (26) does not have this symmetry. However, for the gauge choices $g_1 = g_2 = \ldots = g_{L/2} = \pm 1$, this invariance is recovered and we obtain the same dimensions as in the $(S, S') = (\frac{1}{2}, 1)$ Heisenberg model studied in section 3.

The eigenenergies in the sectors with $g_l = -1$ of the AB_2 model with periodic ends will correspond to the composition of energies of the $(\frac{1}{2}, 1)$-Heisenberg chains with free boundary conditions and different lattice sizes. This exact correspondence, together with the relation (12), implies that the lowest energy in these sectors, in the bulk limit, will have a finite gap when compared with the ground-state energy, which happens in the sector $g_1 = g_2 = \ldots = g_{L/2} = 1$. This gap is proportional to the surface energy f_∞ of the related $(S, S') = (\frac{1}{2}, 1)$ Heisenberg chain. This produces the interesting feature that the correlation functions of operators which commute with (26) will have a power-law decay with exponents like those of the periodic $(\frac{1}{2}, 1)$-Heisenberg chain, while correlations of non-commuting operators may exhibit an exponential decay, with rate proportional to f_∞. An example of such operators is $\sigma_k^z \sigma_k^+ \sigma_l^-$ where k and l are indices inside a given rectangle in figure 2(*b*) and $\sigma^\pm = \sigma^x \pm \mathrm{i}\sigma^y$. Apart from these pathological correlations most of them will be of the same nature as those of the $(S, S') = (\frac{1}{2}, 1)$ Heisenberg model and our results of section 3 indicate that they are described by a Gaussian-like field theory in the regime $1 > \Delta > -1$.

5. Conclusions

Anisotropic quantum chains with one kind of spin S exhibit a critical phase with continuously varying exponents governed by a $c = 1$ Gaussian-like conformal field theory. This phase starts at the ferromagnetic point $\Delta = 1$ with an endpoint at $\Delta = \Delta_c(S)$, which for half-odd-integer S is expected to be 1 and $\Delta_c(S) > -1$ otherwise. This means that the antiferromagnetic point has quite different physics depending on the parity of $2S$. In this paper we analyse anisotropic Heisenberg chains with two kinds of exchange-coupled centres. Due to a non-compensation effect, these models show ferrimagnetism instead of antiferromagnetism. As we change the anisotropy we move from the ferromagnetic $(\Delta = 1)$ to the ferrimagnetic $(\Delta = -1)$ point. We studied, by finite-size calculations and conformal invariance, four models of this kind; the (S, S')-mixed Heisenberg chains with $(S, S') = (\frac{1}{2}, 1)$ and $(S, S') = (\frac{1}{2}, \frac{3}{2})$, given in equation (1) and the Heisenberg models with XXZ interactions in the lattices of figures 2(*a*) and (*b*) (models ABC and AB_2). We calculated the bulk and surface exponents of the first two models and the bulk exponents of the last two.

All the models we studied show the universal feature of having a critical phase for $1 > \Delta > -1$ with long-distance physics governed by a $c = 1$ Gaussian-like conformal field theory. The critical exponents, along this phase, are model-dependent continuous functions of the anisotropy. The sound velocity and compactification radius of the Gaussian theory go to zero at the isotropic ferromagnetic $(\Delta = 1)$ and ferrimagnetic $(\Delta = -1)$ points. This reflects the fact that at both points we should expect the appearance of quadratic dispersion relations. We strongly believe that this is the general scenario for arbitrary Heisenberg chains showing ferrimagnetism instead of antiferromagnetism.

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