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Critical and off-critical properties of the XXZ chain in external homogeneous and staggered magnetic fields

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Abstract. The phase diagram of the XXZ chain is calculated under the influence of homogeneous and staggered magnetic fields. The model has a rich phase structure with three types of phases. A fully ferromagnetic phase, an antiferromagnetic phase and a massless phase with partial ferromagnetic and antiferromagnetic order. This massless phase's critical fluctuations are governed by a conformal field theory with central charge $c = 1$. When the σ^z-anisotropy Δ is zero the model is exactly integrable through a Jordan–Wigner fermionization and our results are analytic. For $\Delta \neq 0$ our analysis is done numerically using lattice sizes up to $M = 20$. Our results show that for $-1 \leqslant \Delta < \sqrt{2}/2$ the staggered magnetic field perturbation is relevant, whereas for $\sqrt{2}/2 < \Delta \leqslant 1$ it is irrelevant. In the region of relevant perturbations, we show that the massive continuum field theory associated with the model, has the same mass spectrum as the sine–Gordon model.

1. Introduction

The anisotropic $S = \frac{1}{2}$ Heisenberg model, or XXZ chain, is one of the most studied quantum spin system in statistical mechanics. Since its exact solution by Yang and Yang [1], this model has been considered to be the classical example of the success of the Bethe ansatz. The XXZ chain gives us the first example of a critical line with critical exponents varying continuously with the anisotropy. More recently [2, 3] with the advance of the conformal invariance ideas [4], the whole operator content of this model was obtanied. The critical fluctuations along this critical line are governed by a conformal field theory with conformal anomaly $c = 1$ and, moreover, the underlying currents satisfy a $U(1)$ Kac–Moody algebra [5].

The effect of a uniform magnetic field in the phase diagram of the XXZ chain [6] (see figure 1) is to extend the critical phase over a finite region delimited by the critical Pokrovsky–Talapov line (PT line in figure 1) [7], where the chain becomes fully ferromagnetic. Finite-size studies of this extended massless phase [8] showed that it is also described by a $c = 1$ theory with critical exponents now depending on the anisotropy and magnetic field. In the antiferromagnetic region ($\Delta < -1$ in figure 1), where the model is massive (non-critical), an increasing magnetic field increases it destroying the massive phase, which again becomes massless.

Since the uniform magnetic field does not destroy the exact integrability of the quantum chain, the eigenspectra in the whole extended massless phase can be computed exactly.

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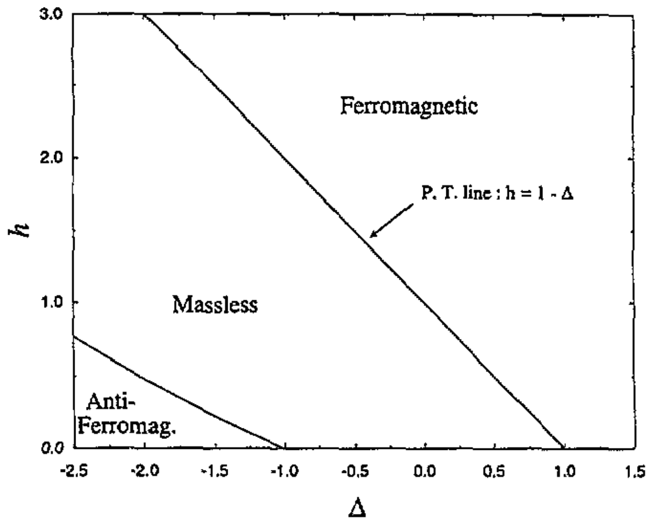

Figure 1. Phase diagram of the Hamiltonian $H(\Delta, h, h_s)$ given in (1) for $h_s = 0$. The different phases and the Pokrovsky–Talapov line are indicated.

This is not the case when we introduce other perturbations, like a thermal perturbation (which is related to a dimerization of the model) or a staggered magnetic field, where exact integrability is lost. Some years ago den Nijs [9], exploring the connection between the eight-vertex and the Gaussian model, conjectured that a staggered magnetic field could be a relevant or irrelevant perturbation depending upon the anisotropy strength. Consequently, in the region where this last perturbation is relevant we should expect an effect opposite to that of a uniform magnetic field, since it will bring the system into a massive phase. Motivated by this, in this paper we study the phase diagram and critical properties of the XXZ chain, when both magnetic fields are present. The XXZ Hamiltonian with these fields is given by

$$H(\Delta, h, h_s) = -\tfrac{1}{2} \sum_{i=1}^{M} \left[\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z + 2\big(h + (-1)^i h_s\big)\sigma_i^z\right] \tag{1}$$

where σ_i^x, σ_i^y and σ_i^z, $i = 1, 2, \ldots, M$ are Pauli matrices attached at the M sites of the chain, Δ is the σ^z-anisotropy parameter and h, h_s are the uniform and staggered fields, respectively. In this paper we treat $H(\Delta, h, h_s)$ with periodic boundary conditions, the lattice size M being an even number.

Using all the machinery coming from finite-size scaling [10] and conformal invariance [4], we will calculate the critical lines, exponents as well as the masses appearing in the underlying massive field theory generated by relevant perturbations.

The paper is organized as follows. In section 2 we review the conformal invariance relations relevant for our purposes and the operator content in the absence of magnetic fields. In section 3 we consider the cases, where $h_s \neq 0$. Initially we discuss the XY chain, where $\Delta = 0$. This case is special since the eigenspectra can be calculated analytically through a Jordan–Wigner fermionization of the Hamiltonian. The general situation where $\Delta \neq 0$ is studied numerically. In section 4 we conclude with a general discussion of our results.

2. Conformal invariance relations and the operator content when $h_s = 0$

Like most statistical mechanical systems in 1+1 dimensions we assume, that the Hamiltonian (1) in its massless regime is conformally invariant. Under this assumption for each operator [4, 11] O_α with dimension x_α and spin s_α in the operator algebra of the infinite system, there exists an infinite tower of states in the quantum Hamiltonian, for a periodic chain of M sites, whose energy and momentum as $M \to \infty$ are given by

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

and

$$P^{\alpha}_{j,j'}(M) = \frac{2\pi}{M}(s_\alpha + j - j') \tag{3}$$

where $j,\, j' = 0, 1, \ldots$; $E_0(M)$ is the ground-state energy and v is the velocity of sound, which can be determined by the dispersion relation of the spectra or by the difference among energy levels belonging to the same conformal tower.

The conformal anomaly c can be obtained from the finite-size corrections of the ground-state energy. For periodic chains, the ground-state energy behaves asymptotically as [12]

$$\frac{E_0(M)}{M} = e_\infty - \frac{\pi c v}{6M^2} + o(M^{-2}) \tag{4}$$

where e_∞ is the ground-state energy per site in the bulk limit. In the case of the XXZ Hamiltonian with no external fields, $H(\Delta, h = 0, h_s = 0)$ and $-1 \leqslant \Delta \leqslant 1$ these relations give us the whole operator content of the underlying field theory [2, 3, 5]. Along the critical line $-1 \leqslant \Delta \leqslant 1$ the central charge is $c = 1$ and the anomalous dimensions appearing in the model are given by integer numbers or by

$$x_{n,m} = n^2 x_p + \frac{m^2}{4x_p} \tag{5}$$

where $x_p = (\pi - \cos^{-1}(-\Delta))/2\pi$ and n and m are integers. Moreover, we can show [5], by combining the integer dimensions with (5), that the model is governed by a conformal field theory satisfying a larger algebra than the Virasoro conformal algebra, namely, a $U(1)$ Kac–Moody algebra. This $U(1)$ symmetry comes from the commutation of the Hamiltonian (1) with the z component of the total spin [13]

$$S_z = \tfrac{1}{2}\sum_{i}^{M} \sigma_i^z = n\,. \tag{6}$$

For a given sector of the Hilbert space where the total spin $S_z = n$ it corresponds to a set of primary operators $O_{n,m}$ with dimensions $x_{n,m}$ ($m = 0, \pm 1, \pm 2, \ldots$) and the number of descendants operators (with dimensions $x_{n,m} + j + j'$, $j, j' \in \mathcal{Z}$) will be given by the product of two $U(1)$ Kac–Moody characters [5]. The operators $O_{n,m}$ can be interpreted, in a Gaussian language [14], as operators with vorticity n and spin wave excitation number m. The critical exponents are obtained from the dimensions (5).

All the above results were obtained for $h_s = h = 0$ and by exploring the exact integrability of the model through the Bethe ansatz, which numerically [2] or analytically [3] produced very precise results. Such integrability is not destroyed by the introduction of the uniform magnetic field and precise results can also be obtained in this case. In the case where $h_s = 0$ and $h \neq 0$, as we see in figure 1, the massless line extends forming a massless phase. This massless phase is ordered ferromagnetically and for a given value of the anisotropy Δ the magnetization changes from zero to its maximum value where the system is fully ordered. The points, where the magnetization reaches its maximum value, form the Pokrovsky–Talapov transition line [7], which separates the massive fully ferromagnetic phase from the massless partially ordered ferromagnetic phase.

The physical mechanism producing the extended massless phase in figure 1 is due to the following. From equations (1) and (6) the magnetic field only decreases the eigenenergies in the sectors where $n > 0$. On the critical line $-1 \leqslant \Delta \leqslant 1$ and $h = 0$ the ground state belongs to the sector $n = 0$. Since we have no gap, a small but finite positive magnetic field will lead the ground state into a sector with $n > 0$, producing a partially ordered ferromagnetic phase. However, the fluctuations around this ordered phase are of a same nature as those appearing in the absence of the magnetic field ($h = 0$). This argument implies that in the whole massless phase we should expect a $c = 1$ Gaussian field theory with the anomalous dimensions like those given in (5). In fact this was observed analytically [8] for $-1 \leqslant \Delta \leqslant 1$ and numerically [15] in the whole extended phase. In [8], although a closed analytic form for the dimensions in the extended massless phase was not derived, the dimensions were shown to be of Gaussian type as in (5), but with x_p now depending on Δ and h. The case where $\Delta = 0$ is special since only in this case the dimensions do not depend on the magnetic field h.

The finite-size analysis of the Hamiltonian (1) with a non-zero uniform magnetic field deserves some comments, since for a fixed value of h the ground-state sector changes as the lattice size increases. In order to approach the bulk-limit physics ($M \to \infty$) correctly we should keep the magnetization per particle fixed for finite chains. This implies that, for a given magnetic field, only a sequence of lattice sizes producing a fixed magnetization, related to h, should be used.

The transition line of Pokrovsky–Talapov type in figure 1 is obtained by calculating the lowest value of the magnetic field where the ground state is ferromagnetic (sector $n = M/2$). This magnetic field is $h = 1 - \Delta$ for arbitrary values of the lattice size M.

3. Results for $h_s \neq 0$

We now analyse the situation, where both magnetic fields h and h_s are non-zero. For $h = 0$ the staggered magnetic field produces an antiferromagnetic ordered ground state. As for $h_s = 0$ the ground state belongs to the sector with $n = 0$. Irrespective of the h_s value we do expect that for sufficiently large values of h ($h \gg h_s$) the same mechanism discussed in last section, which changes the ground-state sector, will also take place. Consequently, we should have a phase transition surface of Pokrovsky–Talapov type, where the ground state becomes the fully ordered ferromagnetic state. The magnetic field $h(\Delta, h_s)$ at this surface, as in the previous section, is calculated by imposing the ground state as the fully ordered ferromagnet state,

$$h(\Delta, h_s) = h_c^{\mathrm{PT}} = \sqrt{h_s^2 + 1} - \Delta\,. \tag{7}$$

For $h > h_c^{\mathrm{PT}}$ the ground state of $H(\Delta, h, h_s)$ is the ferromagnetic state.

3.1. $\Delta = 0$

In this case the Hamiltonian $H(\Delta, h, h_s)$ can be diagonalized through a Jordan–Wigner transformation (see appendix A of [16]):

$$H(0, h, h_s) = \sum_{-\pi \leqslant k \leqslant \pi} \left(2\theta_k \sqrt{h_s^2 + \cos^2 k}\right) \eta_k^\dagger \eta_k - 2nh \tag{8}$$

where η_k are fermionic annihilation operators of momentum k and $\theta_k = 1$ for $-\pi/2 \leqslant k \leqslant \pi/2$ and $\theta_k = -1$ otherwise†. For simplicity we consider the lattice, whose size M is a multiple of 4, and momenta taking the possible values

$$(2l + \epsilon(n))\frac{\pi}{M} \qquad l = -\tfrac{1}{2}M, -\tfrac{1}{2}M + 1, \ldots, \tfrac{1}{2}M - \epsilon(n) \tag{9}$$

where $\epsilon(n) = 1$ or 0 depending if the sector n is even or odd, respectively. The lowest eigenstate in a given sector with $U(1)$ charge n has zero momentum and energy

$$E_n = 2 \sum_{l=-M/4+n/2+(1-\epsilon)/2}^{M/4-n/2-(1+\epsilon)/2} \sqrt{h_s^2 + \cos^2\left(\frac{\pi}{M}(2l + \epsilon)\right)} - 2nh\,. \tag{10}$$

From equation (7) we know that at $h = \sqrt{h_s^2 + 1}$ the system undergoes a phase transition to the ordered ferromagnetic state. In order to detect other phase transitions let us calculate the mass gap of $H(0, h_s, h)$ for small values of h. In such cases the ground state remains in the sector $n = 0$ and the first excited state in the sector $n = 1$. From equation (10) the mass gap is given by

$$G = \lim_{M\to\infty} (E_1 - E_0) = 2(h_s - h)\,. \tag{11}$$

Therefore, as long as $h_s > h$ the model is massive and ordered antiferromagnetically. At $h = h_s$ the model becomes massless and by the same mechanism discussed in the last section, we expect that, as h increases, the model stays massless, until the Pokrovsky–Talapov line is reached. This intermediate phase has a ferromagnetic order, since now the ground state changes sectors as h increases. In figure 2 we show the phase diagram at $\Delta = 0$.

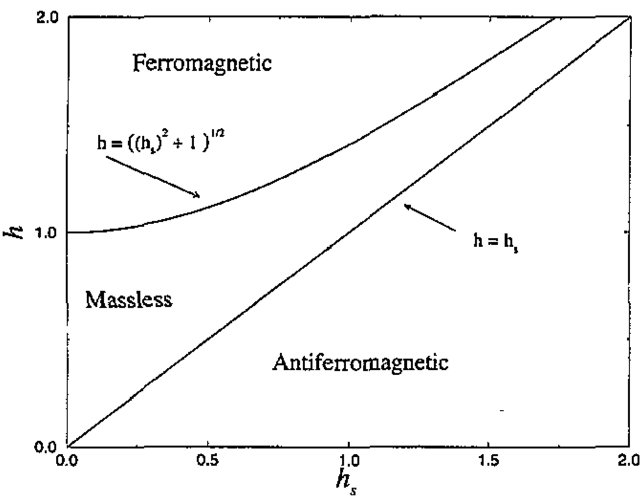

Figure 2. Phase diagram of the Hamiltonian $H(\Delta, h, h_s)$ given in (1) for $\Delta = 0$. The massless phase is separated from the ferromagnetic phase by the Pokrovsky–Talapov line $h = \sqrt{h_s^2 + 1}$ and from the antiferromagnetic phase by the line $h = h_s$.

† In the derivation of (8) the sign θ_k can be arbitrary. With our choice all the excitations are combinations of particles.

Intermediate phase at $\Delta = 0$. In order to analyse this phase using finite-size scaling we should keep the magnetization per particle μ fixed. This is done by choosing a sequence of lattice sizes $M_1, M_2, \ldots$ and sectors $n_1, n_2, \ldots$, such that $\mu = n_i/M_i$, $i = 1, 2, \ldots$ is fixed. For a given lattice size M_i and magnetization μ the magnetic field that gives the ground state in the sector where $n_i = \mu M_i$ should be in the range $h_{\min}(M_i, \mu) \leqslant h \leqslant h_{\max}(M_i, \mu)$, where $h_{\min}(M_i, \mu) = (E_{n_i} - E_{n_i-1})/2$ and $h_{\max}(M_i, \mu) = (E_{n_i+1} - E_{n_i})/2$. From equation (10) in the bulk limit we obtain

$$h_{\min}(\infty, \mu) = h_{\max}(\infty, \mu) = h_\mu = \sqrt{h_s^2 + \sin^2\alpha} \tag{12}$$

where $\mu = n_i/M_i$ and $\alpha = \mu\pi$. Consequently, if the applied field has the value $h = h_\mu$, all the finite lattice sequences M_i $(i = 1, 2, \ldots)$ will have its ground state in the sector with $U(1)$ charge $n_i = \mu M_i$ $(i = 1, 2, \ldots)$. It is simple to verify from (10) that for arbitrary values of $0 \leqslant \mu \leqslant 1$ the gap vanishes as $M \to \infty$, and consequently this partially ordered phase is critical.

For fixed values of μ the finite-size correction of the ground-state energy $E_{\mu M}^{\mathrm{GS}}$ in the asymptotic regime $M \to \infty$ can be obtained using the Euler–Maclaurin formula [17] in (10), which gives us

$$\frac{E_{\mu M}^{\mathrm{GS}}}{M} = e_\infty - \frac{\pi}{6M^2}\frac{\sin(2\alpha)}{h_\mu} + \mathrm{o}(M^{-2}) \tag{13}$$

where

$$e_\infty = -\frac{2}{\pi}\int_0^\alpha \sqrt{h_s^2 + \cos^2 t}\,\mathrm{d}t - 2h_\mu\mu \tag{14}$$

is the energy per particle in the bulk limit $M \to \infty$. The low-lying excited states with non-zero momentum are calculated by changing the fermions momenta entering in the ground state. From these energies we can derive the dispersion relation and the sound velocity

$$v = \frac{\sin(2\alpha)}{h_\mu} \tag{15}$$

which changes continuously along the massless phase. By comparing (13) and (15) with (4) we see that the conformal anomaly is $c = 1$ for all values of μ.

From equation (2) the anomalous dimensions of the conformal operators are calculated from the finite-size corrections to the mass gap amplitudes. For a certain fermionic configuration, they are calculated straightforwardly by using the Euler–Maclaurin formula. For an arbitrary, but rational magnetization $\mu = p/q$ (or magnetic field $h = \sqrt{h_s^2 + \sin^2\mu}$), the lattice sequence with size $M_i = iq$ $(i = 1, 2, \ldots)$ will have its ground state in the $U(1)$ sector $n_i = \mu M_i = ip$ $(i = 1, 2, \ldots)$. The lowest eigenstate in neighbouring sectors where $n_i' = n_i + \bar{n}$ $(\bar{n} = \pm 1, \pm 2, \ldots)$ has zero momentum and will give the mass gap

$$E_{n_i'} - E_{n_i}^{\mathrm{GS}} = \frac{2\pi}{M} v \frac{\bar{n}^2}{4} + \mathrm{o}(M^{-1})\,. \tag{16}$$

The excited states in the sectors n_i' $(i = 1, 2, \ldots)$, obtained by the addition (subtraction) of a momenta $j2\pi/M$ $\left(j'2\pi/M\right)$ to the fermions with positive (negative) momenta, will give us an eigenstate with momentum

$$P_{n_i'}^{j,j'} = \frac{2\pi}{M}(j - j') \tag{17}$$

and mass gap

$$E_{n_i'}^{j,j'} - E_{n_i'}^{\mathrm{GS}} = \frac{2\pi}{M} v\left(\tfrac{1}{4}\bar{n}^2 + j + j'\right) + \mathrm{o}(M^{-1})\,. \tag{18}$$

The relations (2) and (3) enable us to identify the eigenenergies $E_{n_i'}^{j,j'}$ as the conformal tower of the primary operator with dimension $x_{\bar{n},0} = \frac{1}{4}\bar{n}^2$.

Other excited states in the sectors where $n_i' = n_i + \bar{n}$ ($\bar{n} = \pm 1, \pm 2, \ldots$) are derived from the fermion configuration producing $E_{n_i'}^{j,j'}$. These eigenenergies are obtained by replacing fermions with positive (negative) momenta by fermions with negative (positive) momenta. The momenta of such states are

$$P_{n_i',\bar{m}}^{j,j'} = 2\pi\mu + \frac{2\pi}{M}(\bar{n}\bar{m} + j - j') \tag{19}$$

and the mass gaps are

$$E_{n_i',\bar{m}}^{j,j'} - E_{n_i}^{\mathrm{GS}} = \frac{2\pi}{M} v \left(\bar{n}^2 x_{\mathrm{p}} + \frac{\bar{m}^2}{4x_{\mathrm{p}}} + j + j' \right) + \mathrm{o}(M^{-1}) \tag{20}$$

where x_{p} and $\bar{n}, \bar{m}, j, j' = 0, \pm 1, \pm 2, \ldots$. From relations (2) and (3) we identify (20) as the conformal tower of the primary operator with dimension $x_{\bar{n},\bar{m}} = \left(\frac{1}{4}\bar{n}^2 + \bar{m}^2\right)$. Following the discussion of section 2 (see equation (5)) we can interpret $x_{\bar{n},\bar{m}}$ as the dimension of a Gaussian operator $O_{\bar{n},\bar{m}}$ with vorticity $\bar{n}$ and spin-wave number $\bar{m}$. Furthermore, from the degeneracies of the low-lying energies in the conformal towers $\{E_{n_i',\bar{m}}^{j,j'}\}$ we verify that they are given by the product of the characters of the $U(1)$ Kac–Moody algebra as discussed in section 2 for the case where $h_{\mathrm{s}} = 0$. Therefore the whole massless regime has the same critical nature as in the case where $h_s = 0$, being governed by a $c = 1$ conformal field theory with operators satisfying a $U(1)$ Kac–Moody algebra.

Comparing equations (20), (15) and (5) we see that the sound velocity depends on h and h_{s}, while the dimensions $x_{\bar{n},\bar{m}}$ are constants. As we shall see, this independence of exponents is a particular feature of the case where $\Delta = 0$. It is interesting to observe that, contrary to standard conformal towers appearing in critical systems, equation (19) tells us that the eigenstates in the conformal tower have a macroscopic momenta as long as $\mu \neq 0$. This is due to the fact that the fluctuations ruling the critical behaviour are on top of a partially ordered ferromagnet state. Another delicate point appearing here [18] is that a continuum conformal theory can only be constructed for $h = \sqrt{h_{\mathrm{s}}^2 + \sin^2\mu}$, with μ having a rational value, since the lattice sizes and sectors appearing in the finite-size sequences are integer values $\mu = n_i/M_i$ ($i = 1, 2, \ldots$). For h connected with an irrational value of μ, we can only obtain a conformal theory by approximating μ by a close rational number.

Massive phase at $\Delta = 0$. The antiferromagnetic phase for $h < h_{\mathrm{s}}$ is massive with a mass gap given by (11). A continuum field theory describing the physics in this massive phase can be obtained in the neighbourhood of the perturbing parameter $\delta = h_{\mathrm{s}} - h \gtrsim 0$. Such a field theory will be massive and the masses can be estimated from the finite-size behaviour of the eigenspectra. The mass spectrum can be calculated by applying the scheme followed by Sagdeev and Zamolodchikov [19] in the study of the Ising model in an external magnetic field. To do such calculations we should initially find the finite-size corrections of the zero-momenta eigenenergies $E_k(\delta, M)$, $k = 1, 2, \ldots$, at the conformal invariant point $\delta = 0$. In the case of the Hamiltonian (1) the results of [2] tell us that such corrections, not only at $\Delta = 0$ but for arbitrary values of Δ ($-1 \leqslant \Delta \leqslant 1$), are mainly governed by the irrelevant operator with dimension $\bar{x} = x_{0,2} = 1/x_{\mathrm{p}}$ and the descendent of the identity operator with dimension 4. From [2] we have

$$E_k(\delta=0,M)=e_\infty M+\frac{2\pi v}{M}\left(x_k-\frac{c}{12}\right)+a_1\left(\frac{1}{M}\right)^3+a_2\left(\frac{1}{M}\right)^{\bar{x}-1}$$
$$+a_3\left(\frac{1}{M}\right)^{2\bar{x}-3}+a_4\left(\frac{1}{M}\right)^{3\bar{x}-5}+\cdots \tag{21}$$

where x_k is one of the dimensions (5) associated to E_k, and $a_1, a_2, \ldots$ are M-independent factors. According to the scheme of [19], if the perturbed operator which produces the massive behaviour has dimension y, we should calculate the eigenspectra in the asymptotic regime $\delta \to 0$, $M \to \infty$, with

$$X=\delta^{1/(2-y)}M \tag{22}$$

kept fixed. In this regime (21) is replaced by

$$E_k(\delta,M)=e_\infty M+\delta^{1/(2-y)}F_k(X)+\delta^{(\bar{x}-1)/(2-y)}G_k(X)+\delta^{(2\bar{x}-3)/(2-y)}V_k(X)$$
$$+\delta^{(3\bar{x}-5)/(2-y)}H_k(X)+\cdots . \tag{23}$$

The masses of the continuum field theory are obtained from the large-X behaviour of the function [19] $F_k(X)$, i.e.

$$m_k \sim F_k(X)-F_0(X). \tag{24}$$

Equations (21)–(24) can be used for arbitrary Δ. In fact once we know $\bar{x}=1/x_p$, the dimension associated to the off-critical perturbation y as well the generated masses can be calculated from (22)–(24).

In the case $\Delta=0$ the perturbing parameter is $\delta=h_s-h \gtrsim 0$. By keeping $X=(h_s-h)^{1/(2-y)}M$ fixed, with y unknown, we obtain from (10), for $h_s \to 0$

$$E_1-E_0 \approx 2(h_s-h)-\frac{\Omega}{X}h_s^{1/(2-y)} \tag{25}$$

where Ω is a constant. Consequently by comparing (25) with (23) and (24) we obtain the dimension $y=1$ for the perturbing operator and the mass $m_1=2$ associated with the first gap.

The gap associated with the lowest eigenenergy in the sectors with n even is obtained from (10)

$$E_n-E_0=4\sum_{l=1}^{n/2}\sqrt{h_s^2+\sin^2\left[\frac{\pi}{X}(2l-1)h_s^{1/(2-y)}\right]}. \tag{26}$$

Since n is finite, expanding for small values of h_s we get, by comparing with (23), the dimension $y=1$ for the perturbing operator and

$$F_n(X)-F_0(X)=4\sum_{l=1}^{n/2}\sqrt{1+\frac{\pi}{X}(2l-1)^2} \tag{27}$$

which gives, for $X \to \infty$, the masses $m_n=n2=nm_1$. The same result is also obtained in the case where n is odd. Similar calculations for zero-momentum (modulo π) excited states show us that these states are associated with multiples of the mass m_1. However, our calculations show the existence of two equal masses in the system: $m_1=m_2=2$. This is in agreement with the two-fold degeneracy of the first excited state with zero momentum (modulo π) in the ground-state sector $n=0$. The levels are related to the threshold energy $2m_1$.

The dimension $y=1$ for the perturbing operator and the Gaussian dimensions given in (5), with $x_p=\frac{1}{4}$, indicate that this operator is the $O_{0,1}$ operator (see section 2) with dimension $y = x_{0,1} = 1$. This implies that in the region where $x_{0,1} > 2$, ($\Delta > \sqrt{2}/2$) this perturbation will be irrelevant and the phase stays massless after the introduction of a small h_s.

3.2. $\Delta \neq 0$

In this case the analytical diagonalization done for $\Delta = 0$ does not work since the Jordan–Wigner transformation applied to the Hamiltonian (1) will generate a four-body fermionic interaction. Consequently we will resort to numerical analysis. According to finite-size scaling theory (FSS) [10] the critical surfaces of $H(\Delta, h, h_s)$ [10] can be obtained from the extrapolation ($M \to \infty$) of the sequences $(\Delta^{(M)}, h^{(M)}, h_s^{(M)})$ ($M = 2, 4, \ldots$), obtained by solving the equation

$$MG_M(\Delta, h, h_s) = (M-2)G_{M-2}(\Delta, h, h_s) \tag{28}$$

where $G_M(\Delta, h, h_s)$ is the gap of the Hamiltonian (1) with M sites.

In order to simplify our analysis let us consider initially the plane $h = 0$. The critical surface is obtained by solving (28) with Δ or h_s fixed. In tables 1 and 2 we show some of the finite-size sequences for lattice sizes up to $M = 18$. In table 1 h_s is fixed while in table 2 Δ is fixed. In figure 3 we show the curves in the space (Δ, h), that solve (28) for several lattice sizes. We clearly see in the figure that as ($M \to \infty$) the curves for $\Delta < \Delta^* \approx 0.7$ tend toward $h_s = 0$, while for $\Delta > \Delta^*$ the curves tend toward non-zero values of h_s. The blown up region $\Delta \approx \Delta^*$ is also included in figure 3, where the points we used to draw the continuum curves are also shown. These results clearly indicate that for $\Delta < \Delta^* \approx 0.7$ the perturbation introduced by h_s is relevant producing a massive antiferromagnetic phase, while for $1 > \Delta > \Delta^*$ the model stays massless until it reaches a critical staggered field $h_s^* = h_s^*(\Delta)$ which depends on the value of Δ. This is in complete agreement with predictions considering the $\Delta = 0$. There we associated the operator with dimension $x_{0,1} = 1/x_p = \pi/[2(\pi - \cos^{-1}(-\Delta))]$ with the staggered field

Table 1. Sequences of estimators for the anisotropy Δ in the plane $h = 0$, obtained by solving (28) with h_s kept fixed.

$M-2, M$	$h_s = 0.01$	$h_s = 0.03$	$h_s = 0.05$	$h_s = 0.1$	$h_s = 0.2$	$h_s = 0.5$	$h_s = 1.0$
8, 10	−0.454 073 1	−0.015 944 2	0.310 000 8	0.596 932 5	0.761 405 7	0.986 409 1	1.362 844 3
10, 12	−0.350 780 5	0.231 194 9	0.464 232 2	0.659 196 2	0.785 517 0	0.993 019 7	1.363 426 5
12, 14	−0.205 281 8	0.372 466 1	0.544 173 9	0.693 141 4	0.799 615 7	0.997 282 8	1.366 045 7
14, 16	−0.045 778 0	0.457 038 5	0.592 240 8	0.714 569 7	0.808 895 7	1.000 244 5	1.365 056 3
16, 18	0.089 117 0	0.512 236 9	0.624 258 3	0.729 391 6	0.815 491 5	1.002 400 8	1.365 759 2

Table 2. Sequences of estimators for the anisotropy Δ in the plane $h = 0$, obtained by solving (28) with Δ kept fixed.

$M-2, M$	$\Delta = 0.6$	$\Delta = 0.65$	$\Delta = 0.675$	$\Delta = 0.7$	$\Delta = 0.725$	$\Delta = 0.75$	$\Delta = 0.8$
8, 10	0.101 037 6	0.121 390 5	0.134 410 5	0.149 907 1	0.168 248 6	0.189 089 0	0.242 044 4
10, 12	0.077 625 5	0.095 840 1	0.107 885 9	0.122 570 5	0.140 485 5	0.162 175 7	0.217 677 9
12, 14	0.062 430 0	0.078 960 4	0.090 177 9	0.104 146 5	0.121 597 6	0.143 258 4	0.200 506 5
14, 16	0.051 830 2	0.066 915 0	0.077 375 3	0.090 641 2	0.107 564 9	0.129 051 7	0.187 588 5
16, 18	0.044 053 2	0.057 897 5	0.067 676 3	0.080 276 1	0.096 652 2	0.117 878 7	0 177 395 6

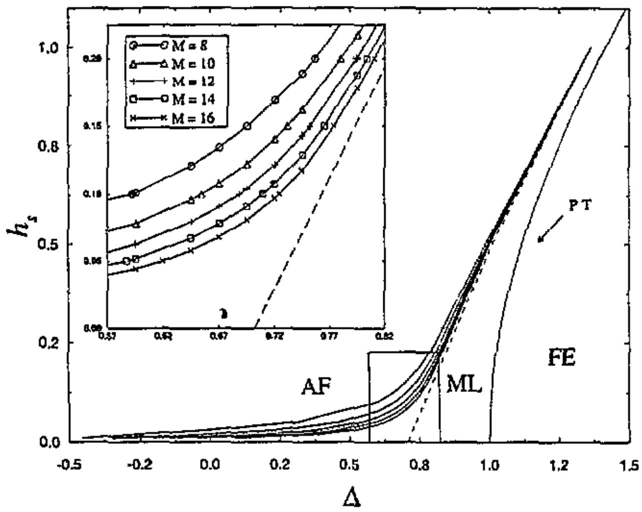

Figure 3. Finite-size estimators of the phase diagram of the Hamiltonian $H(\Delta, h, h_s)$ given in (1) for $h = 0$. The curves are obtained by solving (28) for lattice size pairs $(M-2, M)$ $(M = 10, 12, \ldots, 18)$. The antiferromagnetic, massless and ferromagnetic phases are indicated by AF, ML and FE, respectively. The Pokrovsky–Talapov curve PT is also indicated. The blown-up region $0.57 \leqslant \Delta \leqslant 0.82$ is also shown with the points used to draw the continuum curves.

perturbation. Therefore the perturbation is irrelevant for $\Delta > \Delta^* = \sqrt{2}/2 \approx 0.707$ and the phase, which appears for $\Delta > \Delta^*$ in figure 3, should be a massless antiferromagnetic ordered phase, since $h_s \neq 0$ there. This agrees completely with predictions made in an earlier work by den Nijs [9]. The massless phase (denoted by ML in figure 3) is separated from the fully ferromagnetic phase (denoted by FE in figure 3) by the Pokrovsky–Talapov curve (PT) $h_s = \sqrt{\Delta^2 - 1}$, obtained from (7).

We confirmed numerically the massless nature of the ML phase. Using relations (2)–(4) we verified that the whole phase is governed by a $c = 1$ Gaussian conformal field theory with dimensions as in (5), with x_p varying continuously in the whole phase. As a consequence of (5), ratios of dimensions like $x_{n,0}/x_{1,0} = n^2$ should be independent of x_p. In order to illustrate this let us consider the ratio G_2/G_1 between the gaps in the sectors $n = 2$ and 1. Since the gaps are related to the dimensions $x_{2,0}$ and $x_{1,0}$, this ratio should tend to the value $x_{2,0}/x_{1,0} = 4$, as $M \to \infty$. In figure 4 we show these ratios as a function of Δ for $M = 20$ and some values of h_s. It is clear from this figure that the ratio does indeed change to the expected value of 4, for values of Δ which depend on h_s, consistent with the results shown in figure 3.

Our results also show that the PT curve of figure 3 has a behaviour different from the rest of the Pokrovsky–Talapov surface (7), since it is only along this curve that we have a first-order phase transition. When $h = 0$, crossing the PT curve, the ground state changes from the ferromagnetic sector $n = M/2$ to the sector $n = 0$ discontinuously. As a consequence the magnetization per lattice point changes discontinuously from 1 to zero, as we move from the FE phase to the ML phase (see figure 3). Similarly the staggered magnetization

$$\langle S_z^* \rangle = \tfrac{1}{2}\left\langle \sum_{i=1}^{M} (-)^i \sigma_i^z \right\rangle \tag{29}$$

changes discontinuously from zero to a finite value, which depends on Δ. Also along

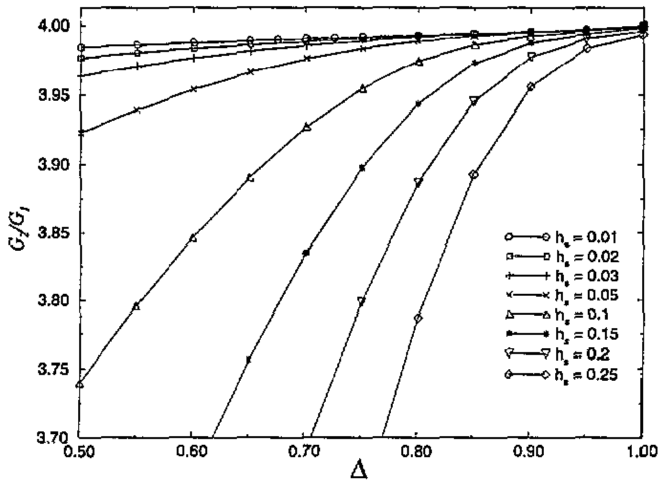

Figure 4. Ratios G_2/G_1 between the gaps G_2 in sector $n = 2$ and G_1 in the sector $n = 1$ of the Hamiltonian $H(\Delta, 0, h_s)$ given in equation (1). The ratios are shown as a function of Δ for lattice size $M = 20$ and some values of h_s. In the region where the phase is massless, we expect the Gaussian relation $G_2/G_1 \to x_{2,0}/x_{1,0} = 4$ as $M \to \infty$.

the surface PT the ground-state wavefunction, which is non-degenerated for $h \neq 0$, becomes M-degenerated when $h = 0$. All the lowest states in the sectors with $n = -\frac{1}{2}M, -\frac{1}{2}M + 1, \ldots, \frac{1}{2}M - 1, \frac{1}{2}M$ become degenerated. We can also show that along this PT curve these degenerated ground-state wavefunctions, for a given sector n, are given exactly by

$$\Psi_n(\Delta, h_s, h = 0) = \sum_{\{s\}}{}' q^{\frac{1}{4}\sum_{i=1}^{M}(-)^i s_i} |s_1, s_2, \ldots, s_M\rangle \tag{30}$$

where

$$\Delta = \sqrt{h_s^2 + 1} = \frac{q + q^{-1}}{2} \tag{31}$$

and $s_i = \pm 1$ $(i = 1, 2, \ldots, M)$ are the eigenvalues in the σ_z basis and the prime in the sum indicates that the configurations $\{s\}$ are constrained to $\sum_{i=1}^{M} s_i = n$.

Massive phase at $\Delta \neq 0$. Similarly, as we did for $\Delta = 0$, let us now investigate the continuum massive field theory describing the fluctuations in the massive phase (AF) of figure 3. The masses of this continuum theory are obtained from the eigenspectrum of the Hamiltonian in the scaling regime given by (22) with $\delta = h_s$ and from our present analysis the dimension y of the perturbing operator is $y = x_{0,1} = \pi/[2(\pi - \cos^{-1}(-\Delta))]$. Using equation (21), (23) and (24) we can calculate the mass ratios of the continuum theory. They are calculated from the asymptotic regime $M \to \infty$ and $X \to \infty$ of the finite-size sequences

$$R_k^{(n)}(X, M) = \frac{F_k^{(n)}(X, M) - F_0^{(0)}(X, M)}{F_1^{(0)}(X, M) - F_0^{(0)}(X, M)} \longrightarrow \frac{m_k^n}{m_0^1}\,. \tag{32}$$

The functions $F_k^{(n)}(X, M)$ are obtained by using in (23) the finite-size sequence of the k zero-momentum states $(k = 0, 1, 2, \ldots)$ in the $U(1)$ sector n. The associated mass

Table 3. The mass-ratio estimators $R_k^{(n)}(X, M)$ defined in (32) for some values of the anisotropy Δ in the plane $h = 0$. The conjectured values of last line are given by (33).

	$\Delta = -\frac{1}{2}$	$\Delta = -\frac{1}{2}\sqrt{2}$		$\Delta = -\frac{1}{2}\sqrt{3}$	
X	m_2/m_1	m_2/m_1	m_3/m_1	m_2/m_1	m_3/m_1
6	1.641 15	1.419 70	2.206 67	1.253 17	2.151 67
10	1.619 67	1.405 02	2.063 04	1.187 85	2.013 52
14	1.622 23	1.405 55	2.030 37	1.152 71	1.997 46
Equation (33)	1.618 03	1.414 21	2.000 00	1.246 98	1.949 86

is $m_k^{(n)}$ while the lightest mass, obtained from the lowest eigenenergy in the sector with $n = \pm 1$, is $m_0^{(1)}$. Our results indicate that for $\Delta \geqslant 0$ we have only two equal masses $M = m_0^{(1)} = m_0^{(-1)}$ and a continuum starting at $2M$. For $\Delta < 0$ other masses appear depending on the value of Δ. In table 3 we present some of our estimators for the mass ratios. We show for $M = 20$ the ratios (32) for some values of X and Δ. There we see two masses $m_1 = m_0^{(1)}$ and $m_2 = m_1^{(0)}$ with ratio $m_2/m_1 = 1.61 \pm 0.03$ for $\Delta = -\frac{1}{2}$. For $\Delta = -\sqrt{2}/2$ ($\Delta = -\sqrt{3}/2$) a third mass appears with the ratios $m_3/m_1 = m_0^{(2)}/m_0^{(1)} = 2.0 \pm 0.2$ $(= 1.9 \pm 0.1)$, $m_2/m_1 = 1.41 \pm 0.01$ $(= 1.2 \pm 0.1)$.

It is well known that the six-vertex model (or the XXZ chain) is transformed into the eight-vertex model (or the XYZ chain) by a thermal perturbation [20]. The spectrum of the transfer matrix of the eight-vertex model was calculated [21] explicitly and is the same as that of the sine–Gordon model [22]. From these results the thermal perturbation in the XXZ chain will produce the following sine–Gordon masses. For $\Delta \geqslant 0$ there will have a mass M twice degenerated plus a continuum starting at $2M$. These are the soliton–antisoliton pair. For $\Delta < 0$, beyond the soliton–antisoliton pair bound states will appear with masses depending on Δ,

$$m_{i+1} = 2m_1 \sin\left(\frac{\pi}{2}\frac{i}{\alpha}\right) \qquad i = 1, 2, \ldots, [\alpha] \tag{33}$$

where

$$\alpha = \frac{3\pi - 4\cos^{-1}(-\Delta)}{\pi} \tag{34}$$

and $[\alpha]$ is the integer part of α.

Our results in table 3 show that in the case where the perturbing field is also the staggered magnetic field, the mass spectrum is the same as the one of sine–Gordon model given by (33) and (34).

4. Conclusions

The results we obtained in the last section enable us to obtain a complete schematic phase diagram of the Hamiltonian (1). For simplicity we only draw it for $\Delta \geqslant 0$ in figure 5. The surface OGFHI separates the antiferromagnetic phase AF from the massless phase ML, while the surface AEDCB separates this last phase from the frozen ferromagnetic phase FE. The order parameters characterizing such phases are the magnetization

$$\overline{M}_h = \left\langle \frac{1}{2}\sum_{i=1}^{M} \sigma_i^z \right\rangle \tag{35}$$

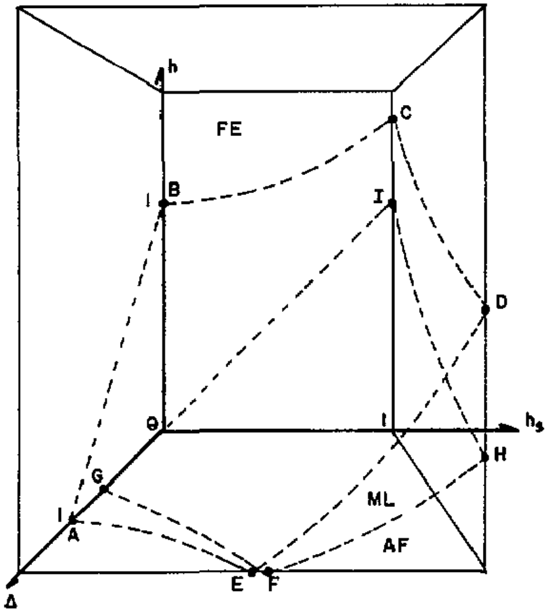

Figure 5. Schematic phase diagram of $H(\Delta, h, h_s)$ given in (1). The phases indicated by FE, ML and AF are the fully ferromagnetic, massless and antiferromagnetic phases, respectively. The Pokrovsky–Talapov surface ABCDE separates the ferromagnetic and massless phases and the surface FGOIH separates this last phase from the antiferromagnetic one. All the phase-transition surfaces are of second order except the line AE where it is first order.

and the staggered magnetization

$$\overline{M}_{h_s} = \left\langle \frac{1}{2} \sum_{i=1}^{M} (-)^i \sigma_i^z \right\rangle. \tag{36}$$

In the FE phase $\overline{M}_h \neq 0$ and $\overline{M}_{h_s} = 0$, in the AF phase $\overline{M}_h = 0$ and $\overline{M}_{h_s} \neq 0$, while for $h \neq 0$ in phase ML we have $\overline{M}_h \neq 0$ and $\overline{M}_{h_s} \neq 0$. At $h = 0$ phases AF and ML have only antiferromagnetic order ($\overline{M}_h = 0$, $\overline{M}_{h_s} \neq 0$), but these phases differ since, contrary to phase AF (or FE), where the correlations have an exponential decay in the massless phase ML the correlations have a power-law decay.

All the phase transition surfaces of figure 5 are of second order, except the curve AE obtained when $h = 0$. The surface AEDCB is the Pokrovsky–Talapov surface given by (7). On this whole surface the ground state is the ordered Heisenberg state with all the spins up, except at the curve AE where t is M degenerated with a wavefunction given exactly by (30).

In the entire massless phase our numerical and analytical results show that the critical exponents change continuously with h, h_s and Δ, except at $\Delta = 0$ where the exponents are constant. The critical fluctuations in this phase are governed by a conformal field theory with central charge $c = 1$ and operators satisfying a $U(1)$ Kac–Moody algebra.

Our numerical and analytical analysis clearly indicates that the staggered magnetic field perturbation is associated with the operator with dimension $x_{0,1} = 1/4x_p = \pi/[2(\pi - \cos^{-1}(-\Delta))]$. This confirms an earlier prediction of den Nijs [9] stating that for $\Delta > \sqrt{2}/2$ this perturbation is irrelevant.

Coming from the massless phase ML to the antiferromagetic phase AF in figure 3, the fluctuations will be ruled by a massive continuum field theory. Our analysis of the last section indicates that such massive field theory is the sine–Gordon field theory with a mass spectrum, which depends on the value of Δ as in (33). This is the same mass spectrum as obtained by perturbing the XXZ by a thermal field.

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