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Integrable spin-$\frac{1}{2}$ *XXZ* Heisenberg chain with competing interactions

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Abstract. The critical behaviour of an integrable model of a spin-$\frac{1}{2}$ chain with nearest-neighbour *XXZ* interaction and a competing three-spin interaction involving nearest and next-nearest neighbours is studied. The phase diagram at zero temperature is obtained. Methods from conformal field theory are used to compute the asymptotics of the spin-spin correlation functions.

1. Introduction

The investigation of exactly solvable models for one-dimensional classical and quantum spin systems has provided the basis for the understanding of the characteristic phenomena occurring in real quasi-one-dimensional magnets. Most of these models describe systems with nearest-neighbour interactions only. An additional interaction involving next-nearest neighbours would allow for the study of the effects of competing interactions such as frustration in these systems. A system that should show such behaviour is given by the following Hamiltonian:

$$\mathcal{H} = \sum_{j=1}^{L} J_1(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) + J_2 \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+2}. \tag{1}$$

For $J_2 = 0$ this model is known to be integrable by Bethe ansatz methods for $S = \frac{1}{2}$ operators S^α [1-3]. However, since this is a singular property of a Hamiltonian the integrability of the system is destroyed by adding the term proportional to J_2. Nevertheless, a few analytical [4, 5] and numerical [6] results exist for the quantum system, giving some insight into the properties of this model: depending on Δ the system is in a gapless spin fluid phase ($|\Delta| < 1$) or an antiferromagnetically ordered Néel phase ($\Delta > 1$) for sufficiently small values of J_2/J_1. For ratios of the exchange couplings greater than some critical value J_c ($J_c \sim 0.3$ for $\Delta = 1$) the ground state of the system shows *dimer* order with a gap for magnon excitations. It remains antiferromagnetically ordered. However, the dominant contribution to the spin-spin correlation function is found at wavenumber $\mathcal{Q} < \pi$ for large J_2. This situation is quite different from the helical phase found in the classical model for $J_2/J_1 > \frac{1}{4}$ ($\Delta = 1$) [7].

Recently, Tsvelik has used the quantum inverse scattering method (QISM) to construct a spin-$\frac{1}{2}$ model that contains a nearest-neighbour Heisenberg exchange term and a competing interaction involving nearest and next-nearest neighbours [8]. Since the relative strength of the Heisenberg coupling and this additional interaction (which will also be denoted by J_2) can be varied without destroying the integrability, this model

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provides a tool to study the effects of competing interactions in much more detail than possible in model (1). Tsvelik has solved this model for certain discrete values of the XXZ anisotropy $\Delta>0$ where the Bethe ansatz simplifies and obtains a qualitative picture of the phase diagram. His basic result is that again there is a phase transition at some critical value of J_2. However, for $J_2>J_c$ the system is not in a massive dimer phase as found for (1) but in a gapless phase with one (two) types of massless magnon excitations for $\Delta>1$ $(0<\Delta<1)$. The ground state carries a finite momentum. The ground state has magnetization $\mathcal{M}=0$ for $0<\Delta<1$ exhibiting long-range antiferromagnetic correlations with wavenumber π for $J_2<J_c$ and in addition at wavenumber $\mathcal{Q}<\pi$ (i.e. incommensurate with the underlying lattice) for $J_2<J_c$. It has finite $\mathcal{M}$ for $\Delta<1$ and $J_2>J_c$ with oscillating spin correlations.

In this paper Tsvelik's analysis is extended to arbitrary $\Delta>-1$ and J_2. The phase boundary is determined and methods from conformal field theory are applied to compute the critical exponents of the model in its critical phases†. In the antiferromagnetic phase at $J_2<J_c$ and in the phase $|\Delta|>1$, $J_2>J_c$ the universality class is that of the Gaussian model or Coulomb gas—characterized by a Virasoro central charge $c=1$. In the antiferromagnetic phase with $J_2>J_c$ the critical theory is given as a product of two Gaussian models, one for each of the two massless magnon excitations. This situation is very similar to that found in certain integrable spin chains with $S>\frac{1}{2}$ [9, 10] and in models of interacting electrons in one spatial dimension [11-13].

The paper is organized as follows. First, a brief review of the construction of the model in the QISM is given and the Bethe ansatz equations that determine the spectrum are written down. Using results from the analysis of the XXZ Heisenberg model [1-3] the critical value of the three-spin coupling is determined for arbitrary $\Delta>-1$ and positive J_2. The characteristics of the various phases are discussed and correlation functions are calculated.

2. Construction of the integrable model

The QISM [14] provides the framework for the construction of integrable models. Central to this construction is the R-matrix which satisfies a Yang–Baxter equation. The R-matrix for the six-vertex model and the related XXZ Heisenberg model is an operator that acts in the product space of two spin-$\frac{1}{2}$ operators $\boldsymbol{S}$ and $\boldsymbol{L}$:

$$R(\lambda)=\frac{1}{\mathrm{i}\sin\gamma}\sinh\frac{\gamma}{2}(\lambda+4\mathrm{i}S^z\otimes L^z)+(S^+\otimes L^-+S^-\otimes L^+)$$

$$=\frac{1}{\mathrm{i}\sin\gamma}\begin{pmatrix}\sinh\frac{\gamma}{2}(\lambda+\mathrm{i}) & 0 & 0 & 0\\ 0 & \sinh\frac{\gamma}{2}(\lambda-\mathrm{i}) & \mathrm{i}\sin\gamma & 0\\ 0 & \mathrm{i}\sin\gamma & \sinh\frac{\gamma}{2}(\lambda-\mathrm{i}) & 0\\ 0 & 0 & 0 & \sinh\frac{\gamma}{2}(\lambda+\mathrm{i})\end{pmatrix}. \qquad (2)$$

Note that at $R(\lambda=\mathrm{i})$ the spins $\boldsymbol{S}$ and $\boldsymbol{L}$ are simply permuted. From R one constructs the monodromy matrix

† In [8] this calculation uses a set of equations in which the interaction between the two magnon branches in the incommensurate antiferromagnetic phase is neglected (see discussion below).

$$T_L(\lambda)=R_1(\lambda)R_2(\lambda)\ldots R_L(\lambda). \tag{3}$$

Here R_j is given by (2) with S^α replaced with S_j^α and the product is taken in the *auxiliary* space of the operators L. The transfer matrix $t_L(\lambda)=\text{trace } T_L(\lambda)$ satisfies $[t_L(\lambda), t_L(\mu)]=0$ and can therefore be considered as a generator for a complete set of commuting operators in the Hilbert space of a spin-$\frac{1}{2}$ chain of length L. From the properties of R it follows that $t_L(\lambda=\mathrm{i})$ is a shift operator, i.e. it shifts a given spin configuration to the left by one site. This suggests a definition of $\mathscr{P}\propto \mathrm{i}\ln t(\lambda=\mathrm{i})$ as the momentum operator of this spin system. The following coefficients of the expansion of $\ln t(\lambda)$ can be identified as Hamiltonian, etc. The first derivative yields the familiar Heisenberg Hamiltonian with XXZ anisotropy†:

$$\mathscr{H}_{XXZ}=\mathrm{i}\frac{\sin\gamma}{\gamma}\frac{\partial}{\partial\lambda}\ln t_L(\lambda)|_{\lambda=\mathrm{i}}=\sum_{j=1}^{L}H_{j,j+1}$$

$$=\sum_{j=1}^{L}(S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+\Delta S_j^zS_{j+1}^z)\qquad \Delta=\cos\gamma. \tag{4}$$

The next integral in this series is found to be

$$\mathscr{I}_2=\mathrm{i}\frac{\sin^2\gamma}{\gamma^2}\frac{\partial^2}{\partial\lambda^2}\ln t_L(\lambda)|_{\lambda=\mathrm{i}}=-\mathrm{i}\sum_{j=1}^{L}[H_{j,j+1},H_{j+1,j+2}]$$

$$=-\sum_{j=1}^{L}\boldsymbol{S}_j\cdot(\boldsymbol{S}_{j+1}\times\boldsymbol{S}_{j+2})\qquad \text{for } \Delta=1. \tag{5}$$

Note that $[\mathscr{H}_{XXZ},\mathscr{I}_2]=0$ by construction. Hence the operator

$$\mathscr{H}=J_1\mathscr{H}_{XXZ}+J_2\mathscr{I}_2 \tag{6}$$

is integrable by Bethe ansatz methods for arbitrary values of J_2/J_1. (In the following I shall set $J_1=1$).

The algebraic Bethe ansatz can be used to study the spectrum of these models. The eigenstates of the transfer matrix $t_L(\lambda)$ with magnetization $\langle\Sigma_j S_j^z\rangle=\frac{1}{2}L-M$ are characterized by a set of M *rapidities* λ_j that have to be chosen such that they satisfy the so-called Bethe ansatz equations

$$\left(\frac{\sin\frac{1}{2}\lambda(\lambda_j+\mathrm{i})}{\sin\frac{1}{2}\gamma(\lambda_j-\mathrm{i})}\right)^L=\prod_{k\neq j}\frac{\sinh\frac{1}{2}\gamma(\lambda_j-\lambda_k+2\mathrm{i})}{\sinh\frac{1}{2}\gamma(\lambda_j-\lambda_k-2\mathrm{i})}. \tag{7}$$

For the energy of the system (6) corresponding to this solution one finds

$$\mathscr{E}=-\sum_{j=1}^{M}\left(1-J_2\frac{\sin\gamma}{\gamma}\frac{\partial}{\partial\lambda_j}\right)\frac{\sin^2\gamma}{\cosh\gamma\lambda_j-\cos\gamma}. \tag{8}$$

2. Phase diagram at $T=0$

2.1. $-1<\Delta=\cos\gamma<1$

The properties of this model for $J_2=0$ have been studied in detail by Takahashi and Suzuki [3]. The solutions of the Bethe ansatz equations (7) are known to be arranged

† In [8] a different normalization of the integrals of motion is chosen: instead of (4) the operator $(\gamma/\sin\gamma)\mathscr{H}_{XXZ}$ is studied. The same difference in the definition of the integral $\mathscr{I}_2$ leads to an additional factor in the amplitude of the three-spin interaction in [8].

in so-called strings—bound states of uniformly spaced complex rapidities with the same real part:

$$\lambda_{\alpha,j}^{(n)} = \lambda_\alpha^{(n)} + \mathrm{i}\left(n+1-2j+\frac{\pi}{2\gamma}(1-v_n)\right) \qquad j=1,\ldots,n. \tag{9}$$

As shown by Takahashi and Suzuki the allowed values of the string lengths n and parities v_n for real γ have to satisfy

$$v_n \frac{\sin\gamma(n-j)\sin\gamma j}{\sin^2\gamma} > 0 \qquad \text{for } j=1,\ldots,n-1. \tag{10}$$

(Note that $n=1$-strings of either parity are allowed.)

In the thermodynamic limit $L\to\infty$ the eigenstates of the system are described by a set of coupled integral equations—one for each allowed string configuration. Fortunately, the analysis of Takahashi and Suzuki shows that most of them have zero energy—their role is mainly to ensure proper counting of the states. In particular, it follows from [3] that at $T=0$ at most 1-strings of parity ± 1 can be present in the ground state configuration.

This allows for the description of the ground state in terms of the energies of these two types of excitations only. They are given in terms of the set of integral equations [3]

$$\begin{aligned} \varepsilon_+(\lambda) &= \varepsilon_+^{(0)}(\lambda) - \int_{\Lambda_+^{(-)}}^{\Lambda_+^{(+)}} \mathrm{d}\mu\, T_+(\lambda-\mu)\varepsilon_+(\mu) + \int_{\Lambda_-^{(-)}}^{\Lambda_-^{(+)}} \mathrm{d}\mu\, T_-(\lambda-\mu)\varepsilon_-(\mu) \\ \varepsilon_-(\lambda) &= \varepsilon_-^{(0)}(\lambda) - \int_{\Lambda_+^{(-)}}^{\Lambda_+^{(+)}} \mathrm{d}\mu\, T_-(\lambda-\mu)\varepsilon_+(\mu) + \int_{\Lambda_-^{(-)}}^{\Lambda_-^{(+)}} \mathrm{d}\mu\, T_+(\lambda-\mu)\varepsilon_-(\mu) \end{aligned} \tag{11}$$

where the bare energies of the 1-strings with positive and negative parity are found from (8) and (9) to be

$$\varepsilon_\pm^{(0)}(\lambda) = \mp\left(1 - J_2 \frac{\sin\gamma}{\gamma}\frac{\partial}{\partial\lambda}\right)\frac{\sin^2\gamma}{\cosh\gamma\lambda_j \mp \cos\gamma} \tag{12}$$

and the phase shift functions are obtained from the Bethe ansatz equations (7)

$$T_\pm(\lambda) = \pm\frac{\gamma\sin 2\gamma}{2\pi\,(\cosh\gamma\lambda_j \mp \cos 2\gamma)}. \tag{13}$$

The integrations in (11) have to be performed over the intervals where $\varepsilon_\pm$ are negative; the boundaries are fixed by the condition $\varepsilon_+(\Lambda_+^{(\pm)})=0$ (and similarly for $\Lambda_-^{(\pm)}$). By Fourier transformation the kernel in (11) can be inverted so that the integration runs over intervals with positive $\varepsilon_\pm$. This procedure leads to the integral equations studied by Tsvelik for $\gamma=\pi/n$ with $n=2,3,\ldots$ [8]. From these equations one finds that for arbitrary values of J_2

$$\begin{aligned} &\varepsilon_-(\lambda)\leqslant 0 \qquad \forall\lambda \qquad \text{i.e. } \Lambda_-^{(\pm)}=\pm\infty \qquad \text{for } \Delta>0 \\ &\varepsilon_+(\lambda)\leqslant 0 \qquad \forall\lambda \qquad \text{i.e. } \Lambda_+^{(\pm)}=\pm\infty \qquad \text{for } \Delta<0. \end{aligned}$$

Hence, one of the unknown functions $\varepsilon_\pm$ can be eliminated from (11).

For $\Delta>0$ the resulting equation is

$$\varepsilon_+(\lambda) = \frac{2\pi\sin\gamma}{\gamma}\left(1 - J_2\frac{\sin\gamma}{\gamma}\frac{\partial}{\partial\lambda}\right) f_+(\lambda) - \int_{\Lambda_+^{(-)}}^{\Lambda_+^{(+)}} \mathrm{d}\mu\, K_+(\lambda-\mu)\varepsilon_+(\mu) \tag{14}$$

where f_+ and K_+ are given in terms of their Fourier transforms as

$$f_+(\omega) = -\frac{\cosh(\pi/\gamma-2)\omega}{\cosh(\pi/\gamma-1)\omega} \qquad K_+(\omega) = \frac{\cosh(\pi/\gamma-3)\omega}{\cosh(\pi/\gamma-1)\omega} \tag{15}$$

ε_- is given in terms of the solution of (14) as

$$\varepsilon_-(\lambda) = \frac{2\pi\sin\gamma}{\gamma}\left(1 - J_2\frac{\sin\gamma}{\gamma}\frac{\partial}{\partial\lambda}\right)f_-(\lambda) - \int_{\Lambda_-^{(-)}}^{\Lambda_+^{(+)}} \mathrm{d}\mu\, K_-(\lambda-\mu)\varepsilon_+(\mu) \tag{16}$$

with

$$f_-(\omega) = \frac{1}{2\cosh(\pi/\gamma-1)\omega} \qquad K_-(\omega) = \frac{\cosh\omega}{\cosh(\pi/\gamma-1)\omega}. \tag{17}$$

For $\Delta < 0$ one can eliminate ε_+ from the integral equations and obtain

$$\begin{aligned}\varepsilon_-(\lambda) &= \frac{2\pi\sin\gamma}{\gamma}\left(1 - J_2\frac{\sin\gamma}{\gamma}\frac{\partial}{\partial\lambda}\right)g_-(\lambda) - \int_{\Lambda_-^{(-)}}^{\Lambda_-^{(+)}} \mathrm{d}\mu\, \bar{K}_-(\lambda-\mu)\varepsilon_-(\mu)\\ \varepsilon_+(\lambda) &= \frac{2\pi\sin\gamma}{\gamma}\left(1 - J_2\frac{\sin\gamma}{\gamma}\frac{\partial}{\partial\lambda}\right)g_+(\lambda) - \int_{\Lambda_-^{(-)}}^{\Lambda_-^{(+)}} \mathrm{d}\mu\, \bar{K}_+(\lambda-\mu)\varepsilon_-(\mu)\end{aligned} \tag{18}$$

with

$$g_-(\omega) = \frac{\cosh(\pi/\gamma-2)\omega}{\cosh(\pi/\gamma-1)\omega} \qquad \bar{K}_-(\omega) = \frac{\cosh(\pi/\gamma-3)\omega}{\cosh\omega}$$

$$g_+(\omega) = \frac{1}{2\cosh\omega} \qquad \bar{K}_+(\omega) = \frac{\cosh(\pi/\gamma-1)\omega}{\cosh\omega}.$$

For the Heisenberg Hamiltonian ($J_2 = 0$) and sufficiently small values of the three-spin coupling, it is known from Takahashi and Suzuki that only 1-strings of positive parity have negative energy, and without an external magnetic field one has $\Lambda_+^{(\pm)} = \pm\infty$. Hence, the energies of the positive-parity 1-strings are found to be

$$\varepsilon_+(\lambda) = -\frac{\pi}{2\gamma}\sin\gamma\left(1 + J_2\frac{\pi}{2}\frac{\sin\gamma}{\gamma}\tanh\frac{\pi\lambda}{2}\right)\frac{1}{\cosh\pi\lambda/2} \tag{19}$$

and the dispersion relation of negative-parity 1-strings is

$$\begin{aligned}\varepsilon_-(\lambda) &= 0 \qquad \text{for } \gamma < \frac{\pi}{2}\\ &= \frac{2\pi}{\gamma}\sin\gamma\left(1 - J_2\frac{\sin\gamma}{\gamma}\frac{\partial}{\partial\lambda}\right)\frac{-\cos\pi^2/2\gamma\cosh\pi\lambda/2}{\cosh\pi\lambda + \cos\pi^2/\gamma} \qquad \text{for } \gamma > \frac{\pi}{2}.\end{aligned} \tag{20}$$

These results hold as long as $\varepsilon_+(\lambda) \leq 0$ and $\varepsilon_+(\lambda) \geq 0$ for all real λ. The value of J_2 where either of these conditions is violated defines the critical value of the three-spin coupling. From (19) we find an upper limit for J_c,

$$J_c = \frac{2\gamma}{\pi\sin\gamma} \tag{21}$$

where 1-strings with zero energy appear at finite λ. For $3\pi/5 < \gamma < \pi$ the critical value of J_2 is defined by the occurrence of negative-parity strings with zero energy (20):

$$J_c = \frac{4\gamma}{\pi\sin\gamma}\sin\frac{\pi^2}{\gamma}\sqrt{\frac{Z-1}{(3-Z)^3}}, \qquad Z^2 = 1 + 4\cos^2\frac{\pi^2}{2\gamma}. \tag{22}$$

Near $\gamma=3\pi/5$, J_c from (21) and (22) varies continuously and $J_c(\gamma\to\pi)=1$ (broken line in Figure 1).

The nature of the new phase with $J_2>J_c$ is easily understood by considering the point $\Delta=0$ (where the *XXZ* model reduces to a system of free fermions). The one-particle dispersion can be found to be

$$\varepsilon(p)=\cos p+\tfrac{1}{2}J_2\sin 2p. \tag{23}$$

In the ground state the negative-energy states

$$\frac{\pi}{2}<p<\frac{3\pi}{2} \qquad \text{for } J_2<J_c=1$$

$$-\frac{\pi}{2}<p<-\frac{\pi}{2}+\mathcal{Q} \qquad \frac{\pi}{2}<p<\frac{3\pi}{2}-\mathcal{Q} \qquad \text{for } J_2>1$$

with $\mathcal{Q}=\cos^{-1}1/J_2$ are filled, allowing for low-lying excitations near the Fermi points at $\pm\pi/2$ and $-\pi/2\pm\mathcal{Q}$, giving two branches of left- and right-moving magnons each.

In addition to the computation of the dispersion of magnon excitations the Bethe ansatz provides information on the density of states. As shown by Tsvelik [8] the system has finite momentum in its ground state for $J_2>J_c$. The magnetization is zero for all values of $|\Delta|<1$ and J_2.

2.2. $\Delta=\cosh\theta\geqslant 1$

For the description of the Ising-like regime one has to replace γ by $\mathrm{i}\theta$ in the equations of the previous section. The thermodynamics of the Heisenberg model ($J_2=0$) in this

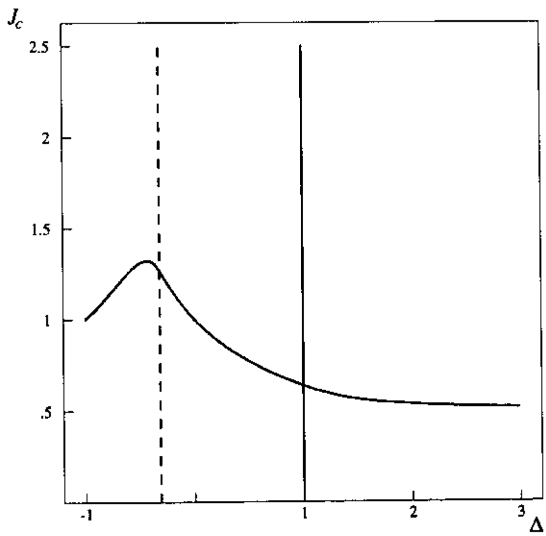

Figure 1. Phase diagram of the Hamiltonian with competing Heisenberg exchange and three-spin interaction (6). The critical value J_c of the three-spin coupling versus anisotropy parameter Δ is shown. For $|\Delta|<1$ and $J_2<J_c$ the system is in a gapless spin liquid phase with long-range antiferromagnetic correlations. The exponents $\eta_\parallel$ and $\eta_\perp$ depend on Δ only. As $J_2>J_c$ a second gapless magnon branch appears, leading to a finite momentum of the ground state and correlations incommensurate with the lattice. For $\Delta>1$ the system undergoes a phase transition from an antiferromagnetically ordered phase for $J_2<J_c$ to a phase with long-range correlations for $J_2<J_c$. The latter are oscillating with a wavenumber incommensurate with the underlying lattice.

regime has been studied by Takahashi [1] for $\Delta = 1$ and Gaudin [2] for $\Delta \geqslant 1$. Again the roots of the Bethe ansatz equations are arranged in strings (9): strings of any length n with positive parity are allowed. The ground state is a sea of 1-strings with energy given by the following integral equation:

$$\varepsilon(\lambda) = \varepsilon^{(0)}(\lambda) - \int_{\Lambda^{(-)}}^{\Lambda^{(+)}} T(\lambda - \mu)\varepsilon(\mu) \qquad -\pi/\theta \leqslant \Lambda^{(\pm)} \leqslant \pi/\theta \tag{24}$$

with

$$\varepsilon^{(0)}(\lambda) = -\left(1 - J_2 \frac{\sinh\theta}{\theta}\frac{\partial}{\partial\lambda}\right)\frac{\sinh^2\theta}{\cosh\theta - \cos\theta\lambda}$$
$$T(\mu) = \frac{\theta}{2\pi}\frac{\sinh 2\theta}{\cosh 2\theta - \cos\theta\lambda}. \tag{25}$$

The integration has to be performed over the interval where $\varepsilon(\lambda) < 0$; the boundaries are fixed by $\varepsilon(\Lambda^{(\pm)}) = 0$. For sufficiently small J_2 one has $\Lambda^{(\pm)} = \pm\pi/\theta$ and the solution of (24) is found by Fourier transformation:

$$\varepsilon(\lambda) = -\frac{K(k)}{\pi}\sinh\theta\left(1 - J_2\frac{\sinh\theta}{\theta}\frac{\partial}{\partial\lambda}\right)\mathrm{dn}\,(K'(k)\lambda|k) \qquad \theta = \pi\frac{K'(k)}{K(k)} \tag{26}$$

($\mathrm{dn}(x|k)$ is the Jacobian elliptic function of modulus k and $K(k)$, $K'(k) = K(k' \times (k' = \sqrt{1-k^2}))$ are the complete elliptic integrals of first kind). For small J_2 the spectrum of magnon excitations has a gap. The critical value of J_2 is defined by the vanishing of this gap, i.e. the appearance of 1-strings with zero energy. After some algebra one finds from (26)

$$J_c = \frac{\pi}{\sinh\theta}\frac{1}{(1-k')K(k)} \tag{27}$$

which decreases monotonically from $2/\pi$ to $\frac{1}{2}$ as θ goes from 0 to ∞, and hence connects smoothly to the result (21) for $\Delta < 1$ (figure 1).

For $J_2 > J_c$ the sea of 1-strings is only partially filled. As a consequence the ground state has a non-zero momentum and aquires a finite magnetization. In the vicinity of the Fermi points massless excitations are possible.

3. Critical exponents

As mentioned above, the system described by the Hamiltonian (6) has massless excitations at zero temperature for $|\Delta| \leqslant 1$ and for $\Delta > 1$, $J_2 > J_c$. Consequently, spin–spin correlation functions show power law behaviour rather than exponential decay in their asymptotics. In recent years, the possibility to compute finite-size corrections to the ground state energy and low-lying excited states in Bethe ansatz systems [15, 16, 9] together with the progress achieved in the understanding of critical phenomena in (1+1)-dimensional quantum systems due to the powerful tool of conformal invariance [17–19] have been used widely to compute the critical exponents associated with these power laws.

In this section these methods shall be used to study asmptotics of the spin–spin correlation functions in system (6). These correlation functions are sums of terms like

$$\langle S^z(x)S^z(0)\rangle \sim \frac{\cos Qx}{|x|^{\eta_\parallel}} \qquad \langle S^-(x)S^+(0)\rangle \sim \frac{\cos Qx}{|x|^{\eta_\perp}} \tag{28}$$

with contributions at different wavenumbers Q.

The critical behaviour in the region $|\Delta|<1$ and $J_2<J_c$ is well understood from studies of the Heisenberg model [20, 16]. All the critical exponents can be given in terms of the 'dressed charge' $Z=\xi(\Lambda_+^\pm)$ with ζ being the solution of the following Bethe ansatz integral equation:

$$\zeta(\lambda)=1-\int_{\Lambda_+^{(-)}}^{\Lambda_+^{(+)}} \mathrm{d}\mu\; T_+(\lambda-\mu)\zeta(\mu) \qquad \Lambda_+^{(\pm)}\to\pm\infty. \tag{29}$$

Using Wiener–Hopf techniques Z can be obtained as

$$Z=\sqrt{\frac{\pi}{2(\pi-\gamma)}} \tag{30}$$

and one finds the dominant terms in the long-distance asymptotic behaviour of the correlators (28) at wavenumber π with exponents $\eta_\parallel=\theta$ and $\eta_\perp=1/\theta$ with $\theta=2Z^2=\pi/(\pi-\gamma)$ independent of J_2.

For $|\Delta|<1$, $J_2>J_c$ there are two branches of massless magnon excitations. This situation is very similar to certain spin chains with $S>\frac{1}{2}$ [9, 10] and the one-dimensional Hubbard model [11, 12]. The energies and momenta of the low-lying excited states of a chain of finite length L are

$$\begin{aligned}\mathscr{E}-\mathscr{E}_0&=\frac{2\pi}{L}(v_+^{(+)}\Delta_+^{(+)}+v_+^{(-)}\Delta_+^{(-)}+v_-^{(+)}\Delta_-^{(+)}+v_-^{(-)}\Delta_-^{(-)})+\mathrm{O}\left(\frac{1}{L}\right)\\ \mathscr{P}-\mathscr{P}_0&=\frac{2\pi}{L}(\Delta_+^{(+)}-\Delta_+^{(-)}+\Delta_-^{(+)}-\Delta_-^{(-)})+\pi\Delta N_++2D_+Q_++2D_-Q_-.\end{aligned} \tag{31}$$

Here $v_+^{(\pm)}(v_-^{(\pm)})$ are the Fermi velocities of right- and left-moving magnon excitations with positive (negative) parity and $Q_+=\pi/2-Q_-\equiv\mathscr{Q}/2$ are the Fermi momenta corresponding to the sea of positive (negative) parity magnons [8]. The critical dimensions $\Delta_\pm^{(\pm)}$ of the primary fields in the critical theory are [18, 12]

$$\Delta_+^{(\pm)}=\frac{1}{2}\left(Z_{++}D_++Z_{-+}D_-\pm\frac{Z_{--}\Delta N_+-Z_{+-}\Delta N_-}{2\det Z}\right)^2$$

$$\Delta_-^{(\pm)}=\frac{1}{2}\left(Z_{+-}D_++Z_{--}D_-\mp\frac{Z_{-+}\Delta N_+-Z_{++}\Delta N_-}{2\det Z}\right)^2$$

determined by the elements of the dressed charge matrix

$$Z=\begin{pmatrix}Z_{++} & Z_{+-}\\ Z_{-+} & Z_{--}\end{pmatrix}=\begin{pmatrix}\xi_{++}(\Lambda_+^{(\pm)}) & \xi_{+-}(\Lambda_-^{(\pm)})\\ \xi_{-+}(\Lambda_+^{(\pm)}) & \xi_{--}(\Lambda_-^{(\pm)})\end{pmatrix} \tag{32}$$

and the integer numbers $\Delta N_\pm$, $D_\pm$. Note that the spin of the states (31) differs from the one of the ground state by $\Delta N_++\Delta N_-$. The elements of the matrix Z are given in terms of the solution of the following set of integral equations:

$$\begin{aligned}
\xi_{++}(\lambda) &= 1-\int_{\Lambda_+^{(-)}}^{\Lambda_+^{(+)}} \mathrm{d}\mu\, T_+(\lambda-\mu)\xi_{++}(\mu)+\int_{\Lambda_-^{(-)}}^{\Lambda_-^{(+)}} \mathrm{d}\mu\, T_-(\lambda-\mu)\xi_{+-}(\mu)\\
\xi_{+-}(\lambda) &= -\int_{\Lambda_+^{(-)}}^{\Lambda_+^{(+)}} \mathrm{d}\mu\, T_-(\lambda-\mu)\xi_{++}(\mu)+\int_{\Lambda_-^{(-)}}^{\Lambda_-^{(+)}} \mathrm{d}\mu\, T_+(\lambda-\mu)\xi_{+-}(\mu)\\
\xi_{-+}(\lambda) &= -\int_{\Lambda_+^{(-)}}^{\Lambda_+^{(+)}} \mathrm{d}\mu\, T_+(\lambda-\mu)\xi_{-+}(\mu)+\int_{\Lambda_-^{(-)}}^{\Lambda_-^{(+)}} \mathrm{d}\mu\, T_-(\lambda-\mu)\xi_{--}(\mu)\\
\xi_{--}(\lambda) &= 1-\int_{\Lambda_+^{(-)}}^{\Lambda_+^{(+)}} \mathrm{d}\mu\, T_-(\lambda-\mu)\xi_{-+}(\mu)+\int_{\Lambda_-^{(-)}}^{\Lambda_-^{(+)}} \mathrm{d}\mu\, T_+(\lambda-\mu)\xi_{--}(\mu).
\end{aligned} \tag{33}$$

In [8] only the diagonal terms in this set of coupled equations are considered. However, the magnon–magnon interaction leads to a mutual deformation of the energy bands for positive- and negative-parity excitations, which is reflected in the structure of (33).

As for the integral equations determining the dressed energies $\varepsilon_\pm$ above, the coupled equations (33) can be reduced to two scalar ones which can be studied using Wiener–Hopf techniques.

For $0<\Delta<1$ one observes that $\Lambda_+^{(+)}=+\infty$. Using this one finds the following result for the dressed charge matrix Z:

$$Z=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0\\ -1 & \sqrt{\pi/\gamma}\end{pmatrix}. \tag{34}$$

Now the critical exponents in (28) can be determined (e.g. see [12]). The states in the spectrum (31) correspond to operators contributing to the long-distance asymptotics of the correlation functions (28). The quantum numbers $\Delta N_\pm$ and $D_\pm$ fix the spin and the momentum of the intermediate state. Hence at wavenumber $Q=\pi(N+D_-)+\mathcal{Q}(D_+-D_-)$ the exponents η are given as

$$\eta=2(\Delta_+^{(+)}+\Delta_+^{(-)}+\Delta_-^{(+)}+\Delta_-^{(-)}) \tag{35}$$

with $\Delta N_+=-\Delta N_-=N$ for $\eta_\parallel=1-\Delta N_-=N$ for $\eta_\perp$. Hence one finds at $Q=\pi(N+D_-)+\mathcal{Q}(D_++D_-)$:

$$\begin{aligned}
\eta_\parallel &= (D_+-D_-)^2+N^2+\frac{\pi}{\gamma}D_-^2\\
\eta_\perp &= (D_+-D_-)^2+N^2+\frac{\pi}{\gamma}D_-^2+\frac{\gamma}{\pi}.
\end{aligned} \tag{36}$$

(In the expression for $\eta_\parallel$ at least one of the integers N and $D_\pm$ has to be non-zero.) As compared to the exponents found for $J_2<J_c$ one observes an enhancement of the longitudinal and suppression of the in-plane correlations at wavenumber π while new contibutions appear at wavenumber $\mathcal{Q}$.

For $-1<\Delta<0$ the dressed charge matrix has the form

$$Z=\begin{pmatrix} \sqrt{\pi/2(\pi-\gamma)} & -\Xi\\ 0 & \Xi\end{pmatrix}. \tag{37}$$

where $\Xi=\xi(\Lambda_-^{(+)})$ is given in terms of the integral equation

$$\xi(\lambda)=1-\int_{\Lambda_-^{(-)}}^{\Lambda_-^{(+)}} \mathrm{d}\mu\, \tilde{K}_-(\lambda-\mu)\xi(\mu). \tag{38}$$

Ξ can be determined in two limiting cases: for $J_2 \to J_c + 0$ one obtains $\Xi = 1$; as $J_2 \to \infty$ one finds $\Lambda_-^{(-)} \to -\infty$. In this limit (38) is of Wiener–Hopf type, giving $\Xi = 1/\sqrt{2}$. For intermediate values of $J_2 > J_c$ the Ξ-dependent elements of the dressed charge matrix vary between these limits, depending on both γ and J_2 through $\Lambda_-^{(\pm)}$. Again, all the critical exponents in (28) are given as function of the elements of Z. Introducing $\theta = 2\Xi^2$ we find at wavenumber $Q = \pi(N + D_-) + \mathcal{Q}(D_+ - D_-)$:

$$
\begin{aligned}
\eta_\parallel &= \theta(D_+ - D_-)^2 + \frac{N^2}{\theta} + \frac{\pi}{\pi - \gamma} D_+^2 \\
\eta_\perp &= \theta(D_+ - D_-)^2 + \frac{N^2}{\theta} + \frac{\pi}{\pi - \gamma} D_+^2 + \frac{\pi - \gamma}{\pi}.
\end{aligned}
\qquad (39)
$$

Again the longitudinal spin correlations with $Q = \pi$ are strongly enhanced while the in-plane ones decay with a larger exponent $\eta_\perp$ when compared to the phase $J_2 < J_c$.

For $\Delta > 1$ and $J_2 > J_c$ one branch of massless magnon excitations is present at $T = 0$, the critical exponent $\eta = 1/(2Z^2)$ as in the first regime ($|\Delta| < 1$, $J_2 < J_c$) with $Z = \xi(\Lambda^{(\pm)})$ and the dressed charge given by the following equation:

$$
\xi(\lambda) = 1 - \int_{\Lambda^{(-)}}^{\Lambda^{(+)}} \mathrm{d}\mu \, T(\lambda - \mu)\xi(\mu). \qquad (40)
$$

The correlators (28) are dominated by the terms at wavenumber π with $\eta_\perp = 1/\theta$ and at wavenumber $\mathcal{Q}$ (twice the Fermi momentum of the magnons) with $\eta_\parallel = \theta$ where $\theta = 2Z^2$. Note that from the considerations above $\frac{1}{2} < \theta < 1$.

4. Discussion

The phase diagram of a spin-$\frac{1}{2}$ chain with *XXZ* Heisenberg exchange and a competing three-spin interaction (6) has been studied in detail. The critical value of the three-spin coupling J_2 has been computed as a function of the *XXZ* anisotropy $\Delta > -1$. The structure of the ground state in the various regions of the phase diagram together with results for the asymptotic behaviour of the spin correlation functions (28) allow for a rather complete picture of the properties of the system:

(i) For $J_2 < J_c$ the properties of the system (6) are essentially unchanged as compared to the *XXZ* Heisenberg model ($J_2 = 0$). In particular, for $|\Delta| < 1$ the critical exponents do not depend on the value of J_2.

(ii) At $J_2 = J_c$ and $\Delta > 1$ the system undergoes a phase transition from a massive phase showing Néel order to a disordered phase with massless excitations. The ground state carries a finite momentum and magnetization and the spin correlations decay as a power law with exponents depending on both J_2 and Δ. The leading contibution to $\langle S^z(x)S^z(0)\rangle$ beyond the constant term is found at a wavenumber $\mathcal{Q} < \pi$.

(iii) For $J_2 > J_c$ and $|\Delta| < 1$ the critical behaviour is characterized by the existence of two branches of massless magnon excitations. The ground state has magnetization $\mathcal{M} = 0$. The spin correlations are antiferromagnetic, incommensurate with the lattice. Longitudinal correlations are enhanced as compared to the phase $J_2 < J_c$.

It should be noted that further integrable multispin interactions can be added to the Hamiltonian (6) by considering the higher conservation laws from the QISM [8]. However, new phases are not likely to be found this way.

In addition to the $T = 0$ properties that have been the focus of this paper the Bethe ansatz provides tools to study the thermodynamics of this system. This is completely analogous to the corresponding problem for the XXZ Heisenberg chain [1-3].

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