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Non-analytic finite-size corrections for the Heisenberg chain in a magnetic field with free and twisted boundary conditions

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Abstract. The finite-size energy spectrum of the anisotropic Heisenberg chain in an external magnetic field is calculated for free and twisted boundary conditions. As with periodic boundary conditions, it is found that the spectra exhibit non-analytical terms which do not fit into the form predicted on the basis of conformal invariance unless extra commensurability conditions between the size of the system and the external field are introduced. Taking these conditions into account some scaling dimensions for associated models are derived.

1. Introduction

The concept of conformal symmetry greatly enhanced the understanding of critical two-dimensional classical and (1+1)-dimensional quantum systems (Belavin *et al* 1984). The conformal anomaly c and the scaling dimensions of the primary conformal order parameters classify the system completely (Friedan *et al* 1984). These critical parameters of the bulk system are directly accessible through the finite-size effects of an affiliated system defined on a strip geometry of infinite length but finite width (Blöte *et al* 1986, Affleck 1986).

This observation led to numerous studies, both numerical and analytical, of the finite-size effects of critical and conformal invariant systems. Much of the analytical work was concerned with the calculation of the conformal anomaly and scaling dimensions of models exactly solvable by the Bethe *ansatz* (BA) method. The prototype of such models is the XXZ chain of N spins $\frac{1}{2}$ with various boundary conditions (Hamer 1986, de Vega and Karowski 1987, Woynarovich and Eckle 1987, Woynarovich 1987, Alcaraz *et al* 1987a,b, 1988, Hamer *et al* 1987, Hamer and Batchelor 1988).

Conformal invariance predicts a so called tower structure (Cardy 1986) for the spectrum of a one-dimensional quantum system, which is given in the most general form (Bogoliubov *et al* 1987) by

$$E_n(N^+,N^-) - E_0 = \frac{2\pi v_{\mathrm{F}}}{N}(x_n + N^+ + N^-) \tag{1.1}$$

$$P_n(N^+,N^-) - P_0 = \frac{2\pi}{N}(s_n + N^- - N^-) + 2Dk_{\mathrm{F}}. \tag{1.2}$$

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The ground-state energy E_0 of the finite system is given by (Blöte *et al* 1986, Affleck 1986)

$$E_0 = N\epsilon_\infty - \frac{\pi v_{\rm F}}{6N}c \tag{1.3}$$

$$E_0 = N\epsilon_\infty + f_\infty - \frac{\pi v_{\rm F}}{24N}c \tag{1.4}$$

for periodic and free boundary conditions, respectively.

Here ϵ_∞ is the ground-state energy density and f_∞ the surface energy of the infinite system, c, x_n and s_n are conformal anomaly, scaling dimensions and spins of the primary scaling operators, $N^{\pm}$ are non-negative integers describing excitations (Woynarovich 1987), D is the number of particles scattered from one Fermi point to the other, P is the momentum of the system and $v_{\rm F}$ is the Fermi velocity. For conformal invariance to hold the latter is required to be the same for all elementary excitations in the system (Woynarovich 1989).

While the predictions of conformal invariance, given in equations (1.1)–(1.4) have been confirmed for a variety of models, it has been observed (Woynarovich *et al* 1989 (hereafter referred to as WET), Woynarovich 1989) that models in the presence of external fields aquire terms in the finite-size corrections of order N^{-1} which are dependent on N itself in a non-analytic way, therefore not fitting into the concept of conformal invariance. Conformal invariance can only be restored if additional commensurability conditions are imposed. The commensurability conditions are connected with the consistent definition of a continuum limit of the *lattice* model which is indispensable for a strict applicability of the concepts of conformal invariance. These aspects have been discussed in detail in WET and we shall not repeat the arguments here.

Alternatively these non-analytic terms have been interpreted as electric and magnetic defects in the incommensurate phase of a two-dimensional model generated from the XXZ chain (Park and Widom 1990a,b).

Similar effects have also been observed in XXZ chains with Dzyaloshinski–Moriya interactions (Alcaraz and Wreszinski 1990), the one-dimensional Bose gas with periodic (WET) and free (reflecting wall) boundary conditions (Berkovich and Murthy 1988b) and most recently the chiral Potts chain (Albertini and McCoy 1990).

The main object of the present work is to show that the effect of external fields in generating non-analytic finite-size corrections to the energy spectra of integrable models is not sensitive to the boundary conditions assumed, but is also present for free and twisted boundary conditions. Therefore it is also possible to generalize surface scaling dimensions and scaling dimensions associated with twisted boundary conditions to the case of non-vanishing external fields.

In the following (section 2) we shall show that the observation of non-analytic terms in the finite-size energy spectra remains true for boundary conditions different from periodic ones. In particular we shall show the presence of non-analytic terms in the finite-size spectrum of the XXZ chain with external magnetic field and free as well as twisted boundary conditions. In section 3 we shall discuss the non-analytic terms briefly for the ground-state energy and evaluate the finite-size spectra to infer surface scaling dimensions and scaling dimensions of associated Ashkin–Teller and q-state Potts quantum chains, the latter related to twisted boundary conditions. Section 4 gives a brief summary.

From the previous work of WET (see also Berkovich and Murthy 1988a,b) it is clear that our results can easily be modified and applied to the one-dimensional Bose gas with a delta-function pair potential.

2. Finite-size energy spectrum

The anisotropic spin-$\frac{1}{2}$ Heisenberg chain of N sites with anisotropy $\cos\gamma$ $(0 \leq \gamma < \pi)$ in an external magnetic field h $(0 \leq h \leq 1+\cos\gamma)$ and with surface fields p and p' at the chain ends

$$\mathcal{H} = \sum_{j=1}^{N'}(-S_j^x S_{j+1}^x - S_j^y S_{j+1}^y + \cos\gamma S_j^z S_{j+1}^z - hS_j^z) + pS_1^z + p'S_N^z - \frac{1}{4}N'(\cos\gamma - 2h) \tag{2.1}$$

is solvable by the Bethe *ansatz* method.

The following special cases of (2.1) have recently been investigated for finite chain length N.

(i) Free $(N' = N-1)$, periodic and twisted $(N' = N,\ p = p' = 0)$ boundary conditions, the latter being defined through

$$S_{N+1}^x \pm \mathrm{i}S_{N+1}^y = \mathrm{e}^{\mathrm{i}\phi}(S_1^x \pm \mathrm{i}S_1^y) \qquad S_{N+1}^z = S_1^z \tag{2.2}$$

without magnetic field $(h = 0)$ (Woynarovich and Eckle 1987, Alcaraz *et al* 1987a,b, 1988, Hamer *et al* 1987, Hamer and Batchelor 1988). These boundary conditions, together with different choices for the surface fields and twist angle have thereby been used to relate (2.1) to Potts and Ashkin–Teller quantum chains and to infer the surface critical behaviour of these models.

(ii) Periodic boundary conditions without surface fields $(p = p' = 0)$, but in the presence of a magnetic field $h \neq 0$ (WET). It was observed that the magnetic field, rendering the number of particles of the ground-state variable, resulted in a structure of the finite-size energy spectrum which was of conformal form only after certain commensurability conditions between the magnetization of the system and the chain length were obeyed. This contrasted the case of zero magnetic field where the ground state is always given by magnetization $\mu = \frac{1}{2}$ and where conformal invariance could immediately be confirmed.

In the following we consider the full Hamiltonian (2.1) with $h \neq 0$ and free and twisted boundary conditions, respectively.

2.1. Free boundary conditions

An eigenstate of (2.1) for free boundary conditions containing M spin waves is completely described by the M parameters λ_j $(j = 1, \ldots, M)$ satisfying the set of algebraic equations (the BA equations) (Hamer *et al* 1987)

$$2N\Phi(\lambda_j, \tfrac{1}{2}\gamma) = 2\pi I_j - \Phi(\lambda_j, \Gamma) - \Phi(\lambda_j, \Gamma') + \sum_{l=1, l\neq j}^{M} (\Phi(\lambda_j - \lambda_l, \gamma) + \Phi(\lambda_j + \lambda_l, \gamma)) \tag{2.3}$$

where

$$\mathrm{e}^{2\mathrm{i}\Gamma} = \frac{p - \Delta - \mathrm{e}^{\mathrm{i}\gamma}}{(p-\Delta)\mathrm{e}^{\mathrm{i}\gamma} - 1} \qquad \mathrm{e}^{2\mathrm{i}\Gamma'} = \frac{p' - \Delta - \mathrm{e}^{\mathrm{i}\gamma}}{(p'-\Delta)\mathrm{e}^{\mathrm{i}\gamma} - 1} \tag{2.4}$$

and

$$\Phi(\lambda, \gamma) = 2\tan^{-1}(\cot\gamma \tanh\lambda). \tag{2.5}$$

Due to the non-zero magnetic field, the number of spin waves $M \neq N/2$ for the ground state, but is rather a free parameter to be fixed by the condition, that the energy

$$E = \sum_{j=1}^{M} \left(h - \frac{\sin^2 \gamma}{\cosh 2\lambda_j - \cos \gamma} \right) - \frac{1}{2}(p + p') \tag{2.6}$$

be minimal with respect to M.

The quantum numbers I_j are given by

$$I_j = j \qquad j = 1, \ldots, M \tag{2.7}$$

(Gaudin 1971, Alcaraz *et al* 1987b).

It should be noted that for free boundary conditions the BA wavefunction has the form of standing waves (Gaudin 1971, Alcaraz *et al* 1987b), therefore the total momentum is always zero. This excludes the possibility of a non-symmetric distribution of roots, as considered in WET for periodic boundary conditions.

In the usual way we introduce a density of roots $\sigma_N(\lambda)$ by

$$z_N(\lambda) = \frac{1}{\pi} \left\{ \Phi(\lambda, \tfrac{1}{2}\gamma) + \frac{1}{2N}[\Phi(\lambda, \Gamma) + \Phi(\lambda, \Gamma') + \Phi(\lambda, \gamma)] - \frac{1}{2N} \sum_{j=-M}^{M} \Phi(\lambda - \lambda_j, \gamma) \right\} \tag{2.8}$$

$$\sigma_N(\lambda) = \frac{\mathrm{d} z_N(\lambda)}{\mathrm{d}\lambda} \tag{2.9}$$

where $\lambda_{-j} = \lambda_j$. Application of the Euler–Maclaurin formula to (2.9)

$$\frac{1}{N} \sum_{\alpha} f(\lambda_\alpha) = \int_{-\Lambda}^{\Lambda} f(\lambda) \sigma_N(\lambda) \, \mathrm{d}\lambda + \frac{1}{24 N^2 \sigma_N(\Lambda)} (f'(-\Lambda) - f'(\Lambda)) + \mathcal{O}(N^{-3}) \tag{2.10}$$

yields the linear integral equation

$$\begin{aligned} \sigma_N(\lambda) = \frac{1}{\pi} \Bigg\{ & \Phi'(\lambda, \gamma/2) + \frac{1}{2N}[\Phi'(\lambda, \Gamma) + \Phi'(\lambda, \Gamma') + \Phi'(\lambda, \gamma) + 2\Phi'(\lambda, 2\gamma)] \\ & - \frac{1}{48 N^2 \sigma_N(\Lambda)} \left(\frac{\mathrm{d}K(\lambda - \Lambda)}{\mathrm{d}\lambda} - \frac{\mathrm{d}K(\lambda + \Lambda)}{\mathrm{d}\lambda} \right) \\ & - \frac{1}{2} \int_{-\Lambda}^{\Lambda} K(\lambda - \lambda') \sigma_N(\lambda') \, \mathrm{d}\lambda' \Bigg\} \end{aligned} \tag{2.11}$$

where $K(\lambda) = \Phi'(\lambda, \gamma)$ is the kernel of the integral equation.

The integration boundary Λ is determined by the sum rule

$$\int_{-\Lambda}^{\Lambda} \sigma_N(\lambda) \, \mathrm{d}\lambda = \frac{2M}{N} + \mathcal{O}(N^{-1}). \tag{2.12}$$

Due to its linearity, the integral equation (2.11) can be solved formally by introducing three new functions which themselves are defined through linear integral equations

$$\sigma(\lambda|\Lambda) = \frac{1}{\pi}\left\{\Phi'(\lambda,\gamma/2) - \frac{1}{2}\int_{-\Lambda}^{\Lambda} K(\lambda-\lambda')\sigma(\lambda'|\Lambda)\,\mathrm{d}\lambda'\right\} \tag{2.13}$$

$$\begin{aligned}\tau(\lambda|\Lambda) = \frac{1}{2\pi}\Big\{&\Phi'(\lambda,\Gamma) + \Phi'(\lambda,\Gamma') + \Phi'(\lambda,\gamma) + 2\Phi'(2\lambda,\gamma)\\ &- \int_{-\Lambda}^{\Lambda} K(\lambda-\lambda')\tau(\lambda|\Lambda)\,\mathrm{d}\lambda'\Big\}\end{aligned} \tag{2.14}$$

$$\rho(\lambda|\Lambda) = \frac{1}{2\pi}\left\{\frac{\mathrm{d}K(\lambda-\Lambda)}{\mathrm{d}\lambda} - \int_{-\Lambda}^{\Lambda} K(\lambda-\lambda')\rho(\lambda|\Lambda)\,\mathrm{d}\lambda'\right\}. \tag{2.15}$$

The formal solution of (2.11) then reads

$$\sigma_N(\lambda) = \sigma(\lambda|\Lambda) + \frac{1}{N}\tau(\lambda|\Lambda) + \frac{1}{24N^2\sigma_N(\Lambda)}[\rho(\lambda|\Lambda) + \rho(-\lambda|\Lambda)]. \tag{2.16}$$

Application of the Euler–Maclaurin formula to the energy (2.6) leads to

$$E = \frac{N}{2}\int_{-\Lambda}^{\Lambda} \epsilon_0(\lambda)\sigma_N(\lambda)\,\mathrm{d}\lambda - \frac{1}{24N\sigma_N(\Lambda)}\frac{\mathrm{d}\epsilon_0(\Lambda)}{\mathrm{d}\Lambda} + E_0 \tag{2.17}$$

$$E_0 = N(-\tfrac{1}{2}\epsilon_0(0) + p + p') \tag{2.18}$$

where the bare energy is given by

$$\epsilon_0(\lambda) = h - \frac{\sin^2\gamma}{\cosh 2\lambda - \cos\gamma}. \tag{2.19}$$

From (2.16) we obtain

$$E = E_0 + N\epsilon\left(\frac{M}{N}\right) + f\left(\frac{M}{N}\right) - \frac{1}{24N}\frac{e(\Lambda)}{\sigma_N(\Lambda)} \tag{2.20}$$

with

$$\epsilon\left(\frac{M}{N}\right) = \frac{1}{2}\int_{-\Lambda}^{\Lambda} \sigma(\lambda|\Lambda)\epsilon_0(\lambda)\,\mathrm{d}\lambda \tag{2.21}$$

$$f\left(\frac{M}{N}\right) = \frac{1}{2}\int_{-\Lambda}^{\Lambda} \tau(\lambda|\Lambda)\epsilon_0(\lambda)\,\mathrm{d}\lambda \tag{2.22}$$

$$e(\Lambda) = \frac{\mathrm{d}\epsilon_0(\Lambda)}{\mathrm{d}\Lambda} + \int_{-\Lambda}^{\Lambda} \rho(\lambda|\Lambda)\epsilon_0(\lambda)\,\mathrm{d}\lambda \tag{2.23}$$

where, of course, $e(\Lambda)$ is also a function of M/N via $\Lambda = \Lambda(M/N)$. We now minimize $E = E(M/N)$, equation (2.20), with respect to M/N, assuming $\mu = \mu(h)$ to be the value where the minimum is taken in the limit $N \to \infty$. By expanding the energy in (2.20) around the minimum, we arrive at the following result for the finite-size energy

$$E(M) = N\epsilon_\infty + f_\infty + \frac{2\pi v_{\rm F}}{N}\left[\frac{1}{(2\xi(\Lambda))^2}(M - N\mu(h))^2 - \frac{1}{48}\right] + \frac{\pi v_{\rm F}^S}{24N^2} + \mathcal{O}(N^{-3}) \tag{2.24}$$

$$\epsilon_\infty = \epsilon(\mu(h)) + \frac{E_0}{N} \tag{2.25}$$

where we have used (2.16) to order N^{-1} to approximate $\sigma_N(\Lambda)$ in (2.20). The consideration of particle-hole excitations (WET, Woynarovich 1989) justifies the definition of two Fermi velocities in (2.24)

$$v_{\rm F} = \frac{e(\Lambda)}{\pi\sigma(\Lambda|\Lambda)} \tag{2.26}$$

$$v_{\rm F}^S = v_{\rm F}\frac{\tau(\Lambda|\Lambda)}{\sigma(\Lambda|\Lambda)}. \tag{2.27}$$

Note that these definitions differ by a factor of $\frac{1}{2}$ from the definition of the Fermi velocities for periodic boundary conditions (WET, Woynarovich 1989). This is due to the differences in the BA equations in the cases of free and periodic (or twisted, see below) boundary conditions.

The quantity $\xi(\Lambda)$, called dressed charge (Korepin 1979, Bogoliubov et al 1986), is given by

$$\xi(\Lambda) = 1 + \frac{1}{2}\int_{-\Lambda}^{\Lambda} \kappa(\lambda|\Lambda)\,{\rm d}\lambda \tag{2.28}$$

where $\kappa(\lambda|\Lambda)$ is defined by the integral equation

$$\kappa(\lambda|\Lambda) = -\frac{1}{2\pi}\left\{[K(\lambda-\Lambda) + K(\lambda+\Lambda)] + \int_{-\Lambda}^{\Lambda} K(\lambda-\lambda')\kappa(\lambda'|\Lambda)\,{\rm d}\lambda'\right\}. \tag{2.29}$$

2.2. Twisted boundary conditions

In the case of twisted boundary conditions the BA equations to be treated for M spin waves described by the parameters λ_j ($j = 1, \ldots, M$) are (Hamer *et al* 1987)

$$N\Phi(\lambda_j, \gamma/2) = 2\pi I_j + \phi + \sum_{l=1}^{M}\Phi(\lambda_j - \lambda_l) \tag{2.30}$$

the quantum numbers I_j being given by

$$I_j = -\frac{1}{2}(M+1) + j \qquad j = 1, \ldots, M. \tag{2.31}$$

Again M is a free parameter to be determined later by minimization of the energy

$$E = \sum_{j=1}^{M}\left(h - \frac{\sin^2\gamma}{\cosh 2\lambda_j - \cos\gamma}\right). \tag{2.32}$$

Instead of quantum numbers (2.31) one could also introduce a non-symmetrical distribution of numbers I_j, i.e. M numbers I_j distributed equidistantly between two numbers I^- and I^+ (WET), resulting from excitations of particles from the left Fermi point to the right one. However, we shall see that the asymmetry already introduced through the twist angle ϕ plays a similar role and the generalization including a non-symmetrical distribution of numbers I_j will be obvious.

As in the case of free or periodic boundary conditions we introduce a root density $\sigma_N(\lambda)$ which satisfies a sum rule

$$\int_{\Lambda^-}^{\Lambda^+} \sigma_N(\lambda)\,\mathrm{d}\lambda = \frac{M}{N} + \mathcal{O}(N^{-1}) \tag{2.33}$$

and which by application of the Euler–Maclaurin formula can be transformed to order N^{-2} in a linear integral equation. The non-symmetrical integration boundaries in (2.33) are due to the translation of quantum numbers I_j by the twist angle ϕ. This non-symmetry can be cast in a second sum rule

$$\frac{1}{2}\left(\int_{\Lambda^+}^{\infty} \sigma_N(\lambda)\,\mathrm{d}\lambda - \int_{-\infty}^{\Lambda^-} \sigma_N(\lambda)\,\mathrm{d}\lambda\right) = -\frac{\phi}{2\pi N}\,. \tag{2.34}$$

These sum rules together with the integral equation for $\sigma_N(\lambda)$, which is formally identical to the one obtained for periodic boundary conditions (see WET), form a closed system and determine completely the state under consideration.

If we replace D by $(-\phi/2\pi)$ in the calculation of WET we can immediately copy the results from that work, namely for the energy

$$E(M,\phi) = N\epsilon_\infty + \frac{2\pi v_\mathrm{F}}{N}\left(\frac{1}{(2\xi(\Lambda))^2}(M - N\mu(h))^2 + (\xi(\lambda))^2\frac{\phi^2}{4\pi^2} - \frac{1}{12}\right) \tag{2.35}$$

and for the momentum

$$P(M,\phi) = -\frac{2\pi}{N}M\frac{\phi}{2\pi}\,. \tag{2.36}$$

Obviously we arrive at the general case discussed above by replacing the term depending on the twist angle by

$$(\xi(\Lambda))^2\left[\frac{\phi^2}{4\pi^2} + D^2\right] \tag{2.37}$$

in the energy (2.35) and

$$-\frac{\phi}{2\pi} + D \tag{2.38}$$

in the momentum (2.36).

3. Ground-state energy and scaling dimensions

We are especially interested in the ground-state energy $E_0(N)$, which can be read off (2.24) and (2.35)

$$E_0(N) = N\epsilon_\infty - \frac{\pi v_\mathrm{F}}{24N}\left[1 - \frac{12}{\xi^2(\Lambda)}(M - \mu(h)N)^2\right] + f_\infty + \frac{\pi v_\mathrm{F}^S}{24N^2} \tag{3.1}$$

for free boundary conditions and

$$E_0(N) = N\epsilon_\infty - \frac{\pi v_\mathrm{F}}{6N}\left[1 - \frac{3}{\xi^2(\Lambda)}(M - \mu(h)N)^2 - 12\xi^2(\Lambda)\frac{\phi^2}{4\pi^2}\right] \tag{3.2}$$

for twisted boundary conditions.

One would now be tempted to infer from (3.1) and (3.2) that the conformal anomaly, which is $c = 1$ in the field free case, has to be modified to read

$$c = 1 - \frac{12}{\xi^2(\Lambda)}m^2 \tag{3.3}$$

in the case of free boundary conditions and

$$c = 1 - \frac{3}{\xi^2(\Lambda)}m^2 - 12\xi^2(\Lambda)\frac{\phi^2}{4\pi^2} \tag{3.4}$$

in the case of twisted boundary conditions, where we have set $m = M - \mu N$. This point of view is advocated in Park and Widom (1990a,b). However, one must observe that the value of c in (3.3) and (3.4) depends on the chain length N via $m = m(N)$ in a non-analytic way, as already discussed in WET. This is clearly against the spirit of the finite-size approach to conformal invariance (Cardy 1986), where the crucial point is to infer the *bulk*, i.e. *size-independent*, conformal or critical parameters of a system from its finite-size behaviour. Therefore we would like to propose† the following interpretation: the energies (3.1) and (3.2) are still not the true ground-state energies of the system, but still exhibit excitations in the form of certain defects. Only if these defects have been removed from the finite system by the commensurability procedure discussed in WET, the *lattice* system aquires a conformal spectrum and is of a form allowing a conformal invariant contiuum limit. Then we have $c = 1$ and also scaling dimensions which are independent of the system size. However, the discussion of the possible defect structure and the related incommensurate phases of models generated by the XXZ chain is of its own value.

Considering the finite-size energies (2.24) and (2.35), we are now in a position to generalize the results of Hamer and Batchelor (1988) for certain scaling dimensions to the case of a non-vanishing magnetic field. For this purpose we briefly rephrase the discussion of WET, how to remove the non-analytic terms in the finite-size energy spectra. For details of the interpretation of this procedure, see WET.

In WET it was argued that, in order to recover the conformal structure of the spectra, one has to choose the value of the magnetic field h in such a way that the magnetization aquires values $\mu(h) = p/q$ with relative prime integers p and q. The

† We would like to thank Professor M N Barber for clarifying discussions about this point.

number of spins in the chain has then to be chosen commensurable with these values of the magnetization, i.e. $N = qN'$ with an integer N'. To obtain the true energy minimum, i.e. the true ground state, the number of spin waves then has to be chosen $M_0 = pN'$.

The general form predicted for the energy gap by conformal invariance (Cardy 1984) is

$$\Delta E = \pi v_{\mathrm{F}} \frac{x_{\mathrm{s}}}{N} \tag{3.5}$$

for free boundary conditions, where x_{s} is the surface scaling dimension. For periodic or twisted boundary conditions, the corresponding relation is (Cardy 1984)

$$\Delta E = 2\pi v_{\mathrm{F}} \frac{x}{N} \tag{3.6}$$

with the scaling dimension x of the associated scaling operator.

Now we calculate the finite-size energy gaps above the true ground state obtained by the described procedure from the finite-size energy spectra (2.24) and (2.35).

For free boundary conditions we obtain from (2.24)

$$\Delta E(\Delta M) = \frac{\pi v_{\mathrm{F}}}{N} \frac{(\Delta M)^2}{2(\xi^2(\Lambda))} \tag{3.7}$$

with $\Delta M = M - M_0$, the number of spin waves excited above the ground state value M_0, revealing the surface scaling dimensions

$$x_{\mathrm{s}}(\Delta M) = \frac{1}{2\xi^2(\Lambda)}(\Delta M)^2. \tag{3.8}$$

In the case of twisted boundary conditions, Hamer and Batchelor (1988) have identified various scaling dimensions for different choices of ϕ, which are associated with the scaling operators of Ashkin–Teller and q-state Potts models. From our general results for the finite-size energy spectrum (2.35) we are able to generalize their results for non-vanishing magnetic field.

Alcaraz *et al* (1987a, 1988) and von Gehlen and Rittenberg (1987) have shown from numerical calculations that the gaps

$$E(\Delta M = 1, \phi = \tfrac{1}{2}\pi) - E(\Delta M = 0, \phi = 0) \tag{3.9}$$

and

$$E(\Delta M = 1, \phi = \tfrac{3}{2}\pi) - E(\Delta M = 0, \phi = 0) \tag{3.10}$$

are associated with the scaling dimensions of the spin-$\frac{1}{4}$ and spin-$\frac{3}{4}$ para-fermion operators for the associated Ashkin–Teller model with periodic boundaries. These quantities are given in our case of $h \neq 0$ from (2.35), (3.9) and (3.10) by

$$x_{\mathrm{pf}}\left(\frac{1}{4}\right) = \frac{1}{(2\xi(\Lambda))^2} + \frac{\xi^2(\Lambda)}{16} \tag{3.11}$$

and

$$x_{\mathrm{pf}}\left(\frac{3}{4}\right) = \frac{1}{(2\xi(\Lambda))^2} + \frac{9\xi^2(\Lambda)}{16} \tag{3.12}$$

generalizing the analytic findings of Hamer and Batchelor (1988) for zero magnetic field.

The scaling dimension of the magnetic operator of the q-state Potts model with periodic boundary conditions (den Nijs 1983, Dotsenko 1984) can be obtained from the gap (Alcaraz *et al* 1987a, 1988)

$$E(\Delta M = 0, \phi = \pi) - E(\Delta M = 0, \phi = 2\gamma) \tag{3.13}$$

with $\cos\gamma = \frac{1}{2}\sqrt{q}$ and have been calculated analytically by Hamer and Batchelor (1988) for $h = 0$. For non-zero magnetic field we obtain from (2.35) and (3.13)

$$x_\sigma = \frac{\pi^2 - 4\gamma^2}{4\pi^2}\xi^2(\Lambda). \tag{3.14}$$

The para-fermion operators of the q-state Potts model with spin $s = \alpha/q$ where $\alpha = 1, \ldots, q-1$ (Fradkin and Kadanoff 1980, Nienhuis and Knops 1985) have corresponding mass gaps (Alcaraz *et al* 1988)

$$E(\Delta M = 1, \phi = 2\pi\alpha/q) - E(\Delta M = 0, \phi = 2\gamma). \tag{3.15}$$

The generalization of the results of Hamer and Batchelor (1988) to non-zero magnetic field can be read off (2.35) and (3.15) to be

$$x_{\mathrm{pf}}(\alpha; q) = \frac{1}{(2\xi(\Lambda))^2} + \frac{\alpha^2\pi^2 - q^2\gamma^2}{\pi^2 q^2}\xi^2(\Lambda). \tag{3.16}$$

In the limit $h \to 0$ Bogoliubov *et al* (1986) have shown that the dressed charge is given by

$$\xi(\Lambda) = \sqrt{\frac{\pi}{2(\pi - \gamma)}} \tag{3.17}$$

(see also Frahm and Yu 1990), therefore all results of Hamer and Batchelor (1988), valid in this limit, can easily be recovered from our general formulae for non-zero magnetic field.

Scaling dimensions for the XXZ chain in a magnetic field and the one-dimensional Bose gas with chemical potential, both with periodic boundary conditions, have already been calculated by Bogoliubov et al (1986), Berkovich and Murthy (1988a,b) and WET. Berkovich and Murthy (1988b) have also calculated surface scaling dimensions for the one-dimensional Bose gas with free (reflecting wall) boundary conditions, but without chemical potential, observing a fractional number of particles which they attribute to a defected ground state of the system. They then further minimize the ground state by subtracting this fractional number of particles, a procedure in perfect accordance to the one we described above for the XXZ chain.

4. Summary

The main result of the present paper is to have demonstrated that the non-analytic finite-size effects in the energy spectrum of the XXZ chain are not sensitive to the boundary conditions assumed. In fact the finite-size energy, given in (2.24) and (2.35), has the same structure for periodic (see WET), free and twisted boundary conditions.

However, it is interesting to observe that in the case of free boundary conditions, there are no non-analytic corrections to the surface energy. Furthermore the twist angle ϕ of twisted boundary conditions plays formally the same role as the number of particles D scattered from one Fermi point to the other.

In WET it was emphasized and also demonstrated in the particular example of the XX chain in a magnetic field that the non-analytic finite-size effects are not consequences of the Bethe-ansatz method, but are present in any system where the ground state depends on external fields such as chemical potential or magnetic field. This observation of course remains true if one investigates different boundary conditions. It is an easy exercise to redo the calculations of appendix 1 of WET for the example of the XX chain with the free and twisted boundary conditions discussed in the present work.

As an application of our calculations and if the commensurability conditions necessary for the spectrum to be of conformal form were obeyed, we were able to infer a number of scaling dimensions for the case of a non-vanishing external field. These scaling dimensions were associated with the boundary conditions we used, namely surface scaling dimensions for the free boundaries and various other scaling dimensions, which were accessible by appropriate choices of the twist angle ϕ in the twisted boundary conditions and which relate to mappings of the XXZ chain to Ashkin–Teller and q-state Potts quantum chains. We expect that it should be possible to calculate scaling dimensions also for other integrable models in external fields.

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