Surface excitations and surface energy of the antiferromagnetic *XXZ* chain by the Bethe ansatz approach

1996 J. Phys. A: Math. Gen. 29 1629

(http://iopscience.iop.org/0305-4470/29/8/011)

J. Phys. A: Math. Gen. **29** (1996) 1629–1638. Printed in the UK

Surface excitations and surface energy of the antiferromagnetic XXZ chain by the Bethe ansatz approach

A Kapustin† and S Skorik‡

† Physics Department, California Institute of Technology, Pasadena, CA 91125, USA
‡ Physics Department, University of Southern California, Los Angeles, CA 90089-0484, USA

Received 17 August 1995, in final form 29 January 1996

Abstract. We study boundary bound states using the Bethe ansatz formalism for the open XXZ ($\Delta > 1$) chain in a boundary magnetic field h. Boundary bound states are represented by the 'boundary strings' similar to those described in Skorik and Saleur. We find that for certain values of h the ground-state wavefunction contains boundary strings and from this infer the existence of two 'critical' fields in agreement with Jimbo *et al*. An expression for the vacuum surface energy in the thermodynamic limit is derived and found to be an analytic function of h. We argue that boundary excitations appear only in pairs with 'bulk' excitations or with boundary excitations at the other end of the chain. We mainly discuss the case where the magnetic fields at the left and the right boundaries are antiparallel, but we also comment on the case of parallel fields. In the Ising ($\Delta = \infty$) and isotropic ($\Delta = 1$) limits our results agree with those previously known.

One-dimensional (1D) integrable quantum field theories with boundary interactions [3] have been intensively studied recently because of their applications in condensed matter physics (see, e.g., [4]). A powerful method for dealing with such problems is the Bethe ansatz, which allows one to extract the basic physical properties from the system of coupled transcendental equations. Among others, it allows one to solve the boundary sine–Gordon model via its lattice regularization, the inhomogeneous XXZ ($|\Delta| < 1$) chain in a boundary magnetic field [1, 5].

In this paper we study the XXZ chain with an even number of spins L in a boundary magnetic field,

$$\mathcal{H} = \tfrac{1}{2}\left\{ \sum_{i=1}^{L-1} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z) + h_1 \sigma_1^z + h_2 \sigma_L^z \right\} \tag{1}$$

in the regime $\Delta > 1$, $h_1 \geqslant 0$, $h_2 \leqslant 0$, focusing on the effects peculiar to systems with boundaries [6]. At $h_1 = h_2 = 0$ this model describes a one-dimensional antiferromagnet with non-magnetic impurities, which are accessible experimentally. We exploit the Bethe ansatz solution for this model, which was first derived in [7], together with the well known results for the periodic chain [8]. We find new 'boundary string' solutions to the Bethe equations, similar to the boundary strings existing in the $|\Delta| < 1$ regime [1]. For certain values of the boundary magnetic field the ground-state configuration contains boundary 1-strings. Boundary excitations are obtained by removing (or adding, depending on the

0305-4470/96/081629+10$19.50

sign of h) boundary strings from the ground-state wavefunction. Their energy was first obtained in [2] by the algebraic approach.

A peculiar feature of the Bethe ansatz solution of the periodic chain is that the excitations (holes in the Dirac sea) appear only in pairs [9]. We argue that similarly the boundary excitations can appear only in pairs with bulk excitations or with boundary excitations at the other end of the spin chain. There is no such restriction in the solution of the semi-infinite chain by the algebraic approach [2].

Using the Bethe ansatz solution we calculate the surface energy (see, e.g., [10]),

$$E_{\mathrm{surf}}(L, \Delta, h) = E_{\mathrm{gr}} - E^0_{\mathrm{gr}} \tag{2}$$

in the thermodynamic limit $L = \infty$. Here E_{gr} is the ground-state energy of (1) and E^0_{gr} is that of the periodic chain. We give an interpretation of our results in the limits $\Delta \to \infty$ and $\Delta \to 1$, corresponding to the 1D Ising and XXX models, respectively. Finally, we comment on the structure of the ground state when the boundary magnetic fields are parallel.

Let us first set up the Bethe ansatz (BA) notations and list the relevant results about the XXZ chain [7, 8]. In [7] the eigenstates of (1) were constructed for arbitrary Δ. As usual in the BA picture, the n-magnon eigenstates $|n\rangle$, satisfying $\mathcal{H}|n\rangle = E|n\rangle$, are linear combinations of the states with n spins down, located at sites $x_1, \dots, x_n$:

$$|n\rangle = \sum f^{(n)}(x_1, \dots, x_n)|x_1, \dots, x_n\rangle.$$

The wavefunction

$$f(x_1, \dots, x_n) = \sum_P \varepsilon_P A(p_1, \dots, p_n) \mathrm{e}^{\mathrm{i}(p_1 x_1 + \dots + p_n x_n)} \tag{3}$$

contains n parameters $p_j \in (0, \pi)$ which are subject to quantization conditions, called Bethe equations (BE):

$$\mathrm{e}^{2\mathrm{i}Lp_j} \frac{\mathrm{e}^{\mathrm{i}p_j} + h_1 - \Delta}{1 + (h_1 - \Delta)\mathrm{e}^{\mathrm{i}p_j}} \frac{\mathrm{e}^{\mathrm{i}p_j} + h_2 - \Delta}{1 + (h_2 - \Delta)\mathrm{e}^{\mathrm{i}p_j}} = \prod_{l \neq j}^{n} \mathrm{e}^{\mathrm{i}\Phi(p_j, p_l)}. \tag{4}$$

The summation in (3) is over all permutations and negations of p_j. The energy and spin of the n-magnon state are given by [7]

$$E = \tfrac{1}{2}[(L-1)\Delta + h_1 + h_2] + 2\sum_{j=1}^{n}(\cos p_j - \Delta) \qquad S_z = \frac{L}{2} - n. \tag{5}$$

It is convenient to rewrite BE using the following mappings,

$$\Delta = \cosh\gamma \geqslant 1 \qquad \gamma \geqslant 0 \tag{6}$$

$$p = -\mathrm{i}\ln\frac{\cosh\frac{1}{2}(\mathrm{i}\alpha + \gamma)}{\cosh\frac{1}{2}(\mathrm{i}\alpha - \gamma)} \tag{7}$$

(our definition of $p(\alpha)$ differs from that of [8] by the shift $\alpha \to \alpha + \pi$ and it was chosen in such a way that $p(\alpha)$ be an odd function that maps $-\pi < \alpha < \pi$ to $-\pi < p < \pi$),

$$h = \cosh\gamma + \frac{\sinh\frac{1}{2}\gamma(1-H)}{\sinh\frac{1}{2}\gamma(1+H)} = \sinh\gamma\coth\tfrac{1}{2}\gamma(H+1) \qquad h_{\mathrm{lim}} < |h| < \infty \tag{8}$$

$$h = \cosh\gamma - \frac{\cosh\frac{1}{2}\gamma(1-H)}{\cosh\frac{1}{2}\gamma(1+H)} = \sinh\gamma\tanh\tfrac{1}{2}\gamma(H+1) \qquad |h| < h_{\mathrm{lim}}. \tag{9}$$

The latter two mappings are defined on $H \in (-\infty, \infty)$ and are necessary to cover the region $-\infty < h < \infty$, with positive h corresponding to $H \in (-1, \infty)$. The value $h_{\rm lim} \equiv h(\infty) = \sinh\gamma$ lies between two critical fields $h_{\rm cr}^{(1)}, h_{\rm cr}^{(2)}$ defined as follows [2]:

$$h_{\rm cr}^{(1)} = \Delta - 1 \qquad h_{\rm cr}^{(2)} = \Delta + 1. \tag{10}$$

Both critical fields correspond to $H = 0$ and the gap $h_{\rm cr}^{(1)} < h < h_{\rm cr}^{(2)}$ corresponds to $0 < H < \infty$. In these notations equation (4) becomes

$$\left[\frac{\cosh\frac{1}{2}(\mathrm{i}\alpha_j + \gamma)}{\cosh\frac{1}{2}(\mathrm{i}\alpha_j - \gamma)}\right]^{2L} B(\alpha_j, H_1) B(\alpha_j, H_2) = \prod_{m\neq j} \frac{\sinh\frac{1}{2}(\mathrm{i}\alpha_j - \mathrm{i}\alpha_m + 2\gamma)\sinh\frac{1}{2}(\mathrm{i}\alpha_j + \mathrm{i}\alpha_m + 2\gamma)}{\sinh\frac{1}{2}(\mathrm{i}\alpha_j - \mathrm{i}\alpha_m - 2\gamma)\sinh\frac{1}{2}(\mathrm{i}\alpha_j + \mathrm{i}\alpha_m - 2\gamma)} \tag{11}$$

where

$$B(\alpha, H) = \frac{\cosh\frac{1}{2}(\mathrm{i}\alpha + \gamma H)}{\cosh\frac{1}{2}(\mathrm{i}\alpha - \gamma H)} \qquad h_{\rm lim} < |h| < \infty \tag{12}$$

$$B(\alpha, H) = \frac{\sinh\frac{1}{2}(\mathrm{i}\alpha + \gamma H)}{\sinh\frac{1}{2}(\mathrm{i}\alpha - \gamma H)} \qquad |h| < h_{\rm lim} \tag{13}$$

are called boundary terms. The energy equation (5) takes the form

$$E = \tfrac{1}{2}[(L-1)\cosh\gamma + h_1 + h_2] - 2\sinh\gamma \sum_{j=1}^{n} p'(\alpha_j) \qquad p'(\alpha) = \frac{\sinh\gamma}{\cosh\gamma + \cos\alpha}. \tag{14}$$

In the thermodynamic limit $L \to \infty$ the real roots α_j of BE form a dense distribution in the open interval $(0, \pi)$ with density $\rho(\alpha)$, $\mathrm{d}I = 2L(\rho + \rho_h)\,\mathrm{d}\alpha$ being the number of roots in the interval $\mathrm{d}\alpha$. The logarithm of equation (11) is

$$2Lp(\alpha_j) + \frac{1}{\mathrm{i}}\ln B(\alpha_j, H_1) + \frac{1}{\mathrm{i}}\ln B(\alpha_j, H_2) + \phi(2\alpha_j) = \sum_{l=1}^{n} \phi(\alpha_j - \alpha_l) + \phi(\alpha_j + \alpha_l) + 2\pi I_j \tag{15}$$

where I_j form an increasing sequence of positive integers, and

$$\phi(\alpha) = -\mathrm{i}\ln\frac{\sinh\frac{1}{2}(2\gamma + \mathrm{i}\alpha)}{\sinh\frac{1}{2}(2\gamma - \mathrm{i}\alpha)} \qquad \phi(0) = 0. \tag{16}$$

Taking the derivative of equation (11) and defining ρ for negative α by $\rho(\alpha) = \rho(-\alpha)$, we obtain

$$p'(\alpha) + \frac{1}{2L}p'_{\rm bdry}(\alpha) = \int_{-\pi}^{\pi} \phi'(\alpha - \beta)\rho(\beta)\,\mathrm{d}\beta + 2\pi(\rho(\alpha) + \rho_h(\alpha)) \tag{17}$$

with

$$p'_{\rm bdry}(\alpha) = -\mathrm{i}\frac{B'(\alpha, H_1)}{B(\alpha, H_1)} - \mathrm{i}\frac{B'(\alpha, H_2)}{B(\alpha, H_2)} + 2\phi'(2\alpha) - 2\pi\delta(\alpha) - 2\pi\delta(\alpha - \pi). \tag{18}$$

The presence of delta-functions in (18) is due to the fact that $\alpha_j = 0$ and $\alpha_j = \pi$ are always solutions to (11), which should be excluded, since they make the wavefunction (3) vanish identically [5].

In equation (17) the 'boundary terms' are down by a factor $1/2L$. Neglecting p'_{bdry} and setting $\rho_h = 0$, we obtain the equation for the ground-state density of the periodic XXZ chain [11]. Solving it by the Fourier expansion

$$f(\alpha) = \sum_{l=-\infty}^{\infty} \hat{f}(l) \mathrm{e}^{\mathrm{i}l\alpha} \qquad \hat{f}(l) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\alpha) \mathrm{e}^{-\mathrm{i}l\alpha} \, \mathrm{d}\alpha \tag{19}$$

and using (14), we recover the result for the ground-state energy of the periodic chain [11]:

$$2\pi \hat{\rho}_{\mathrm{per}}(n) = \frac{\hat{p}'(n)}{1 + \hat{\phi}'(n)} \qquad \hat{\phi}'(n) = \mathrm{e}^{-2\gamma|n|} \qquad \hat{p}'(n) = (-1)^n \mathrm{e}^{-\gamma|n|} \tag{20}$$

$$E_{\mathrm{gr}}^0 = \frac{L\Delta}{2} - 2L \sinh\gamma \int_{-\pi}^{\pi} \rho_{\mathrm{per}}(\alpha) p'(\alpha) \, \mathrm{d}\alpha = \frac{L\Delta}{2} - L \sinh\gamma \sum_{n=-\infty}^{\infty} \frac{\mathrm{e}^{-\gamma|n|}}{\cosh\gamma n}. \tag{21}$$

The spin of the ground state is $S_z = L/2 - L\int_{-\pi}^{\pi} \rho_{\mathrm{per}} \mathrm{d}\alpha = 0$, which is a well known result [11].

An elementary 'bulk' excitation above the vacuum in model (1) is a hole in the distribution of I_j, but only a pair of holes can occur for the periodic chain, as argued in [9]. Thus physical excitations contain an even number of holes. The energy of the hole with rapidity θ can be easily computed,

$$\varepsilon_h(\theta) = \sinh\gamma \sum_{n=-\infty}^{\infty} \frac{(-1)^n \mathrm{e}^{\mathrm{i}n\theta}}{\cosh\gamma n} > 0 \tag{22}$$

and the spin with respect to the vacuum is $S_z = 1/2$. (Our result, equation (22), differs from the conventional one by the shift $\theta \to \theta + \pi$, but the dispersion relation is unchanged by rapidity reparametrization.)

Analogous arguments can be applied to analyse 'bulk' string solutions with complex values of α. Although there exists an infinite hierarchy of complex strings of arbitrary length, and quartets, their energy vanishes with respect to the vacuum [12].

So far we have discussed the bulk excitations, which are essentially the same as in the periodic chain. Let us now turn to the new solutions of equation (11): boundary strings. The analysis is close to that of [1]. Boundary excitations have their wavefunction (3) localized at the left or the right ends of the chain, and in the limit $L \to \infty$ the two ends may be considered separately. Let us first study the left boundary, $h_1 > 0$. The fundamental boundary 1-string consists of one root located at $\alpha_0 = -\mathrm{i}\gamma H_1$ for $0 < h_1 < h_{\mathrm{cr}}^{(1)}$, and at $\alpha_0 = \pi - \mathrm{i}\gamma H_1$ for $h_{\mathrm{cr}}^{(2)} < h_1 < \infty$ (in both cases $-1 < H_1 < 0$). The string is a solution of BE due to the mutual cancellation of the decreasing modulus of the first term in (11) and the increasing modulus of the second term $B(\alpha, H_1)$ as $L \to \infty$ and $\alpha \to \alpha_0$. When $h_{\mathrm{cr}}^{(1)} < h_1 < h_{\mathrm{cr}}^{(2)}$, no such solution exists. Introduction of such a string into the vacuum with the density of roots $\rho(\alpha)$ defined from

$$p'(\alpha) + \frac{1}{2L} p'_{\mathrm{bdry}}(\alpha) = \int_{-\pi}^{\pi} \phi'(\alpha - \beta)\rho(\beta) \, \mathrm{d}\beta + 2\pi\rho(\alpha) \tag{23}$$

leads to the redistribution of roots by $\delta\rho \equiv 2L(\tilde{\rho} - \rho)$, where $\tilde{\rho}$ is the density of real roots in the state with the boundary string. $\delta\rho$ satisfies an integral equation:

$$0 = \int_{-\pi}^{\pi} \phi'(\alpha - \beta)\delta\rho(\beta) \, \mathrm{d}\beta + \phi'(\alpha - \alpha_0) + \phi'(\alpha + \alpha_0) + 2\pi\delta\rho. \tag{24}$$

From the latter we find

$$2\pi\delta\hat{\rho}(n) = -\frac{2\cos n\alpha_0 \mathrm{e}^{-2\gamma|n|}}{1 + \mathrm{e}^{-2\gamma|n|}}. \tag{25}$$

The energy of the boundary 1-string with respect to this vacuum, $\tilde{\varepsilon}_{\mathrm{b}}$, is the difference between the energy of the state with the string and the vacuum energy. Using equation (14), we obtain

$$\tilde{\varepsilon}_{\mathrm{b}} = -2\sinh\gamma p'(\alpha_0) - 2L\sinh\gamma \int_{-\pi}^{\pi} (\tilde{\rho} - \rho) p'(\alpha)\,\mathrm{d}\alpha = -\sinh\gamma \sum_{n=-\infty}^{\infty} \frac{(-1)^n \mathrm{e}^{\mathrm{i}n\alpha_0}}{\cosh\gamma n}. \qquad (26)$$

Similarly, for the spin of the boundary string we obtain $S_z = -1/2$. We see that the energy (26) is negative, so the state described by the root density ρ is not the ground state. The correct ground state wavefunction (3) should contain the boundary 1-string root α_0. The ground-state density $\tilde{\rho}$ in this case satisfies the equation

$$p'(\alpha) + \frac{1}{2L}(p'_{\mathrm{bdry}}(\alpha) - \phi'(\alpha - \alpha_0) - \phi'(\alpha + \alpha_0)) \\ = \int_{-\pi}^{\pi} \phi'(\alpha - \beta)\tilde{\rho}(\beta)\,\mathrm{d}\beta + 2\pi\tilde{\rho}(\alpha). \qquad (27)$$

The boundary excitation is obtained by removing from vacuum the root α_0, which means that it has the energy $-\tilde{\varepsilon}_{\mathrm{b}} > 0$ and spin $1/2$, equal to the spin of the bulk hole. Substituting the value of α_0 into (26), we get the boundary excitation energy, which precisely agrees with the one obtained in [2]:

$$\varepsilon_{\mathrm{b}}(h_1) = \sinh\gamma \sum_{n=-\infty}^{\infty} \frac{(-1)^{\kappa n} \mathrm{e}^{\gamma H_1 n}}{\cosh\gamma n} \qquad -1 < H_1 < 0 \qquad (28)$$

with $\kappa = 1$ if $h_1 < h_{\mathrm{cr}}^{(1)}$ and $\kappa = 2$ if $h_1 > h_{\mathrm{cr}}^{(2)}$.

The above description of the ground state is valid when the boundary 1-string solution exists, that is, when $h_1 < h_{\mathrm{cr}}^{(1)}$ or $h_1 > h_{\mathrm{cr}}^{(2)}$. When the boundary magnetic field approaches $h_{\mathrm{cr}}^{(1)}$ from below or $h_{\mathrm{cr}}^{(2)}$ from above, the boundary string moves towards the real axis, merging with the Dirac sea of real roots. In the regime $h_{\mathrm{cr}}^{(1)} < h_1 < h_{\mathrm{cr}}^{(2)}$ the boundary string solution is non-existent and the correct ground state contains only real roots, whose density ρ is determined by equation (23). Thus in the Bethe ansatz picture the description of the ground state changes discontinuously at $h_1 = h_{\mathrm{cr}}^{(1)}$ and $h_1 = h_{\mathrm{cr}}^{(2)}$. We will see later, however, that observable quantities (e.g., energy and spin) are continuous at these points. Another conclusion is that the boundary bound state is present only for $h_1 < h_{\mathrm{cr}}^{(1)}$ and $h_1 > h_{\mathrm{cr}}^{(2)}$, in complete agreement with [2].

From (22) and (28) we see that for $h_1 < h_{\mathrm{cr}}^{(1)}$ the energy of the boundary excitation is smaller than the bottom of the energy band of bulk excitations and becomes equal to it at $h_1 = h_{\mathrm{cr}}^{(1)}$ (see figure 1). So in this regime we may interpret the boundary excitation as the bound state of the kink, which gets unbound at $h_1 = h_{\mathrm{cr}}^{(1)}$. For $h_1 > h_{\mathrm{cr}}^{(2)}$ the energy of the boundary bound state is bigger than the top of the energy band. Therefore it is stable, in spite of its huge energy.

Besides the fundamental boundary 1-string, there exists an infinite set of 'long' boundary strings, consisting of roots $\alpha_0 - 2\mathrm{i}k\gamma, \alpha_0 - 2\mathrm{i}(k-1)\gamma, \ldots, \alpha_0 + 2n\mathrm{i}\gamma$ with $n, k \geqslant 0$. We will call such solution an (n, k) boundary string (thus the fundamental boundary string considered above is the (0,0) string). One can use the same arguments as given in [1] to show that the (n, k) string is a solution of BE when its 'centre of mass' has positive imaginary part and the lowest root $\alpha_0 - 2\mathrm{i}k\gamma$ lies below the real axis. Thus, sufficiently long boundary string solutions exist even in the region $h_{\mathrm{cr}}^{(1)} < h_1 < h_{\mathrm{cr}}^{(2)}$. However, a direct calculation shows that their energy vanishes with respect to the vacuum, so they represent

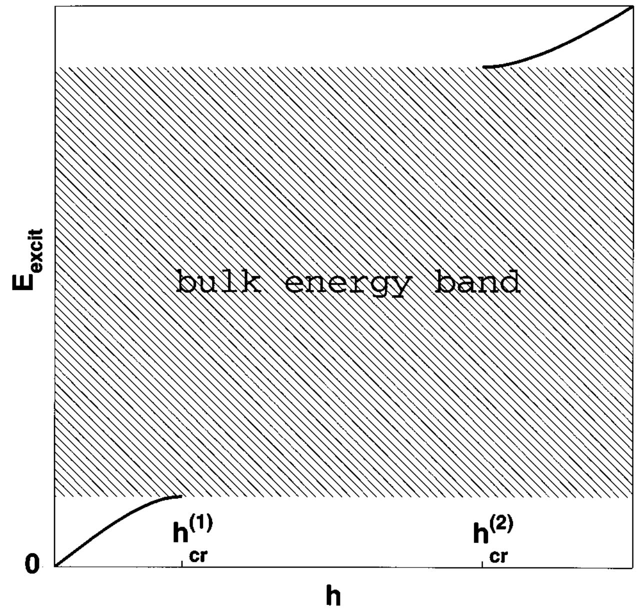

Figure 1. Full curve: a schematic plot of the energy of the boundary excitation, $\varepsilon_b(h)$, as a function of the boundary magnetic field h. Shaded area: the energy band of the bulk excitations.

charged vacua†. (An analogous phenomenon occurs for the 'long' strings in the bulk [12]: if the imaginary part of α lies outside the strip $-2\gamma < \mathrm{Im}\alpha < 2\gamma$, the root α gives no contribution to the energy.) For $0 < h_1 < h_{\mathrm{cr}}^{(1)}$ and $h_{\mathrm{cr}}^{(2)} < h_1 < \infty$, the $(n, 0)$ strings also represent charged vacua, while (n, k) strings with $k \geqslant 1$ have the same energy (28) as the boundary bound state found above, and hence represent charged boundary excitations‡.

Consider now the right boundary, $h_2 < 0$ ($H_2 < -1$). Now the fundamental boundary 1-string solution $\alpha_0 = -\mathrm{i}\gamma H_2$ exists for any value of h_2 in the interval $-h_{\mathrm{lim}} < h_2 < 0$ (respectively $\alpha_0 = \pi - \mathrm{i}\gamma H_2$ for $h_2 < -h_{\mathrm{lim}}$). Explicit calculation shows that it has non-vanishing energy only if $-2 < H_2 < -1$, which corresponds to $-h_{\mathrm{cr}}^{(1)} < h_2 < 0$ (respectively $h_2 < -h_{\mathrm{cr}}^{(2)}$). For such values of h_2, the energy of the 1-string with respect to the vacuum (23) is positive and equal to $\varepsilon_b(-h_2)$ (see equation (28)) and its spin is $S_z = -1/2$. In some sense the pictures are dual for the positive and negative h cases: there exist two states when $|h|$ is not between $|h_{\mathrm{cr}}^{(1)}|$ and $|h_{\mathrm{cr}}^{(2)}|$, one with boundary 1-string and one without. One of them is the ground state and another is the excited state at the boundary, and these states exchange their roles when the sign of h changes. The analysis of long boundary strings is very similar to that at the left boundary, and therefore will be omitted. The net result is again that long boundary strings represent charged vacua or charged boundary excitations.

In all examples shown above, the charge of boundary excitations turned out to be half-integer. One can easily check that this is true for all boundary strings representing charged excitations. Since the charge of physical excitations is obviously restricted to be

† As an example, consider the boundary (1,0) string consisting of the roots $\alpha_0 + 2\mathrm{i}\gamma, \alpha_0$. It exists if $-1 < H_1 < 1$, although the (0,0) string exists only if $-1 < H_1 < 0$. The (1,0) string has charge $S_z = -1$ and vanishing energy with respect to the vacuum.

‡ For example, the (1,1) string with roots $\alpha_0 + 2\mathrm{i}\gamma, \alpha_0, \alpha_0 - 2\mathrm{i}\gamma$ has $S_z = -3/2$ and energy given by (28) with respect to the physical vacuum.

an integer (see (5)), we conclude that a boundary excitation can only appear paired with the bulk excitation of half-integer charge (i.e. containing an odd number of holes) or with a boundary excitation at the other end of the chain. We give a qualitative interpretation of this fact below.

To compute the vacuum surface energy, equation (2), of model (1), one should use equation (14) in the limit $L = \infty$ with the root density determined from equations (23) or (27) and the boundary terms (12) or (13), depending on the value of h. Define for convenience

$$g(\Delta) = \frac{\Delta}{2} + 2\sinh\gamma \sum_{n=1}^{\infty} \frac{e^{-2n\gamma} - 1}{\cosh 2n\gamma}. \tag{29}$$

We consider separately the following intervals for positive h_1 and negative h_2.

(i) $|h_{1,2}| < h_{cr}^{(1)}$. The ground state contains one boundary 1-string, corresponding to h_1. The spin of the ground state can be found to be $S_z = 0$. Using equations (13), (18) and (27), and subtracting the bulk contribution (21), we get

$$E_{surf} = \tfrac{1}{2}(h_1 + h_2) - g(\Delta) - \sinh\gamma \sum_{n=1}^{\infty} (-1)^n \frac{e^{-\gamma H_1 n} - e^{\gamma H_2 n}}{\cosh \gamma n}. \tag{30}$$

(ii) $|h_{1,2}| > h_{cr}^{(2)}$. The ground state contains one boundary 1-string and has $S_z = 0$. From equations (12) and (27) it follows

$$E_{surf} = \tfrac{1}{2}(h_1 + h_2) - g(\Delta) - \sinh\gamma \sum_{n=1}^{\infty} \frac{e^{-\gamma H_1 n} - e^{\gamma H_2 n}}{\cosh \gamma n}. \tag{31}$$

(iii) $h_{cr}^{(1)} < |h_{1,2}| < h_{lim}$. The ground state has no boundary strings and its spin is zero. From (23) and (13) one obtains the same expression as in case (i).

(iv) $h_{lim} < |h_{1,2}| < h_{cr}^{(2)}$. From (23) and (12) one obtains the same expression as in case (ii). The ground state has the same structure as in case (iii).

A qualitative plot of the surface energy as a function of h ($h = h_1 = -h_2$) is given in figure 2. The apparent difference between (30) and (31) is an artefact of our parametrization of h in terms of H. In fact, E_{surf} is an analytic function of h in the domain $h \in (0, \infty)$, which can be seen after substituting H as a function of h according to (8) and (9). In this sense the fields $h_{cr}^{(1,2)}$ are not actually 'critical.' We find for $h_1 = h_2 = 0$ the value

$$E_{surf} = -\frac{\Delta}{2} + 4\sinh\gamma \left(\frac{1}{4} + \sum_{n=1}^{\infty} \frac{e^{2n\gamma} - 1}{1 + e^{4n\gamma}} + \sum_{n=1}^{\infty} \frac{(-1)^n}{1 + e^{2n\gamma}} \right). \tag{32}$$

Note that one can obtain the boundary magnetization $\langle \sigma_1^z \rangle$ [2] immediately from the formula for the surface energy (30) and (31) by differentiating with respect to h_1.

In the extreme anisotropic limit $\Delta \to \infty$, $h \sim \Delta$ of the XXZ chain (1) one gets the one-dimensional Ising model:

$$\mathcal{H} = \tfrac{1}{2} \left\{ \sum_{i=1}^{L-1} \Delta \sigma_i^z \sigma_{i+1}^z + h_1 \sigma_1^z + h_2 \sigma_L^z \right\}. \tag{33}$$

In this limit from (8) and (9) one has

$$h \approx \Delta \pm e^{-\gamma H} \tag{34}$$

and the gap between $h_{cr}^{(1)}$ and $h_{cr}^{(2)}$ disappears, so for any h there exists a boundary bound state. The energy of the 'bulk' hole (22) becomes θ-independent and equal to Δ, since only the $n = 0$ term contributes to the sum when $\gamma \to \infty$. The energy of the boundary bound

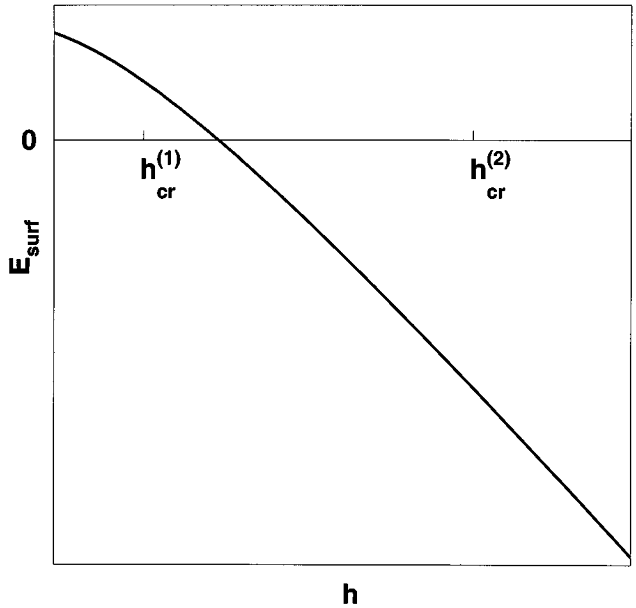

Figure 2. A schematic plot of the vacuum surface energy as a function of the boundary magnetic field $h = h_1 = -h_2$.

state (28) becomes $\varepsilon_b = \Delta \pm e^{-\gamma H_1} = h_1$. This suggests the following interpretation in terms of the Ising chain. In the Ising ground state the ith spin has the value $(-1)^i$. Local bulk excitation of the smallest energy 2Δ can be obtained by flipping one spin (the first and last spins excepted). The arising two surfaces (domain walls) separating the flipped spin from its right and left neighbours are called kinks and carry the energy Δ each. A kink corresponds to a hole in the Bethe ansatz picture and kinks obviously appear only in pairs, which demonstrates that holes can exist only in pairs, too. The charge of the one-spin-flipped state is equal to one, in agreement with the charge of two holes in BA. In addition to charge one excitation, one has charge zero excitation of the same energy obtained by flipping any even number of spins in a row. In the BA this corresponds to the 'two holes and 2-string' state. In the Ising model the left (right) boundary bound state is obtained by flipping the first (last) spin. Such a state has the energy $h_1 + \Delta$ above the vacuum energy, where h_1 is the contribution of the boundary term in (33) and Δ is the energy of the kink created due to the boundary–bulk interaction. Thus flipping the boundary spin actually gives a combination of the boundary excitation and the bulk kink. Still another possibility is to flip all spins, creating two boundary bound states, one at each boundary. This explains why, in the BA picture, a boundary excitation can exist only if paired with a hole in the Dirac sea or with another boundary excitation. The vacuum surface energy (2) of the Ising chain in the thermodynamic limit is $(\Delta - h_1 + h_2)/2$. The $\Delta/2$ contribution here is the bulk interaction energy that we lost when we disconnected the periodic chain and $\pm h_{1,2}/2$ is the contribution of each of the boundary terms. Taking the limit $\gamma \to \infty$ in equations (30) and (31), we obtain the expected result $E_{\text{surf}} \to (\Delta - h_1 + h_2)/2$.

In the isotropic (rational) limit $\Delta \to 1$ (i.e. $\gamma \to 0$) one gets the XXX chain in a boundary magnetic field, which was discussed in the BA framework in [13] for $0 < h_{1,2} < 2$.

From (8) and (9) one has in the limit

$$h = \frac{2}{1+H}. \tag{35}$$

There is only one critical field $h_{\rm cr} = 2$, which is the limit of $h_{\rm cr}^{(2)}$. Passing from summation to integration in equation (31), we obtain for $0 < h_1 < \infty$, $0 < -h_2 < \infty$,

$$\begin{aligned} E_{\rm surf} &= \frac{1}{2}(h_1+h_2) - \frac{1}{2} + \frac{\pi}{2} - \int_0^\infty \mathrm{d}x \, \frac{\mathrm{e}^{-(2/h_1-1)x} - \mathrm{e}^{(2/h_2-1)x} + \mathrm{e}^{-x}}{\cosh x} \\ &= \frac{1}{2}(h_1-h_2) - \frac{1}{2} + \frac{\pi}{2} - \int_0^\infty \mathrm{d}x \, \frac{\mathrm{e}^{-(2/h_1-1)x} + \mathrm{e}^{(2/h_2+1)x} + \mathrm{e}^{-x}}{\cosh x} \end{aligned} \tag{36}$$

where the second line was obtained from the first one after a simple manipulation. This agrees with the results of [13]. For $h_1 = h_2 = 0$ one has from (36) $E_{\rm surf} = (\pi-1)/2 - \ln 2$.

Another aspect is the structure of the ground state in the regime $h_{1,2} > 0$. Assuming that, for example, for $h_{1,2} > h_{\rm cr}^{(2)}$ the ground state contains both left and right boundary 1-strings to minimize the energy, we end up, after a short calculation, with a half-integer spin for the vacuum, which signals that such a state cannot, in fact, be the vacuum. Hence, the ground state must have a more intricate structure. Appealing to the Ising limit $\gamma \to \infty$, one sees that for $h_{1,2} > \Delta$ the ground state must have both boundary spins directed opposite to the magnetic field and, therefore, contain a kink in the bulk (recall that L is even). On the other hand, for $h_{1,2} < \Delta$ the lowest energy configuration is such that the boundary spins are antiparallel, which means that the physical vacuum contains what was once called a boundary excitation at one of the ends. This suggests that for finite Δ the correct ground-state wavefunction of the Hamiltonian (1) should contain a bulk hole with the minimal possible energy (i.e. the kink with zero rapidity $\theta = 0$) and both boundary 1-strings when $h_{1,2} > h_{\rm cr}^{(2)}$. Such a state has zero spin. Changing the rapidity of this stationary kink away from zero, one obtains in such a way an excited state whose energy can be arbitrarily close to the vacuum state, which means that there is a new gapless branch in the spectrum†. Similarly, when $h_{\rm cr}^{(1)} < h_{1,2} < h_{\rm cr}^{(2)}$, for the ground state to have the integer charge it should also contain a kink in the bulk. When $h_{1,2} < h_{\rm cr}^{(1)}$ the physical vacuum contains only one of the two boundary 1-strings and no stationary kink in the bulk (when $h_1 = h_2$ there are two possibilities of having either left or right boundary 1-string in the vacuum, corresponding to the obvious two-fold degeneracy of the Ising ground state in this case). Such a state has a smaller energy for $h_{1,2} < h_{\rm cr}^{(1)}$ than the state with a hole in the bulk and two boundary strings, whereas for $h_{1,2} > h_{\rm cr}^{(2)}$ the state with the bulk hole is energetically preferable, since in this case $\varepsilon_{\rm b} > \varepsilon_h$ (see figure 2 and [2]). This situation is in some sense analogous to the case of the periodic antiferromagnetic XXZ chain with odd L, where the ground state contains a kink. According to the above discussion the surface energy in the case $h_{1,2} > h_{\rm lim}$ is

$$E_{\rm surf} = \frac{1}{2}(h_1+h_2) - g(\Delta) + \varepsilon_h(0) - \sinh\gamma \left(1 + \sum_{n=1}^{\infty} \frac{\mathrm{e}^{-\gamma H_1 n} + \mathrm{e}^{-\gamma H_2 n}}{\cosh \gamma n}\right). \tag{37}$$

In the rational ($\gamma \to 0$) limit $\varepsilon_h(0)$ vanishes and equation (37) becomes

$$E_{\rm surf} = \frac{1}{2}(h_1+h_2) - \frac{1}{2} + \frac{\pi}{2} - \int_0^\infty \mathrm{d}x \, \frac{\mathrm{e}^{-(2/h_1-1)x} + \mathrm{e}^{-(2/h_2-1)x} + \mathrm{e}^{-x}}{\cosh x}. \tag{38}$$

This expression agrees with the one obtained in [13]. Note that the authors of [13] obtained equation (38) under the assumption that $0 < h_{1,2} < h_{\rm cr}$, whereas our derivation shows that

† In the Ising limit $\gamma \to \infty$ the energy of the kink is independent of rapidity and, therefore, this branch degenerates to the vacuum.

this result is valid for $0 < h_{1,2} < \infty$. In the Ising limit equation (37) gives the correct result $E_{\rm surf} = (3\Delta - h_1 - h_2)/2$. Observe that for the XXX chain the following equality holds (see (36) and (38)): $E_{\rm surf}(h_1, h_2) = E_{\rm surf}(h_1, -h_2)$. This is a consequence of the decomposition $E_{\rm surf} = f(h_1) + f(h_2) +$ constant, which takes place in the limit $L = \infty$ when two boundaries are independent, and the obvious property of the semi-infinite chain $f(-h) = f(h)$. The same statements are true for the surface energy of XXZ chain apart from the $\varepsilon_h(0)$ contribution (see (37)).

We would like also to mention that within the BA technique it is also possible to calculate the boundary S-matrix for the scattering of kinks (represented by holes in the Dirac sea) in the ground state of the Hamiltonian (1) or in the excited boundary state. Such a calculation has been performed in [13] for the boundary XXX chain and in [1, 5] for the boundary sine–Gordon model. For the boundary XXZ chain these S-matrices have been obtained by Jimbo *et al* [2] in the algebraic approach.

Acknowledgments

One of the authors (SS) would like to thank H Saleur for helpful discussions. The work of AK was supported in part by the US Department of Energy under grant No DE-FG03-92-ER40701. The work of SS was supported by the grant NSF-PHY-9357207.

References

[1] Skorik S and Saleur H Boundary bound states and boundary bootstrap in the sine–Gordon model with Dirichlet boundary conditions USC-95-01 hep-th/9502011 *J. Phys. A: Math. Gen.* to appear
[2] Jimbo M, Kedem R, Kojima T, Konno H and Miwa T 1995 *Nucl. Phys.* B **441** 437
[3] Ghoshal S and Zamolodchikov A B 1994 *Int. J. Mod. Phys.* A **9** 3841
[4] Kane C L and Fisher M P A 1992 *Phys. Rev.* B **46** 15 233
[5] Fendley P and Saleur H 1994 *Nucl. Phys.* B **428** 681
[6] McCoy B and Wu T 1973 *The Two-Dimensional Ising Model* (Cambridge, MA: Harvard University Press)
[7] Alcaraz F, Barber M, Batchelor M, Baxter R and Quispel G 1987 *J. Phys. A: Math. Gen.* **20** 6397
[8] Gaudin M 1971 *Phys. Rev. Lett.* **26** 1301; *La Fonction d'Onde de Bethe* (Paris: Masson)
[9] Faddeev L D and Takhtajan L A 1981 *Phys. Lett.* **85A** 375
[10] Batchelor M T and Hamer C J 1990 *J. Phys. A: Math. Gen.* **23** 761
[11] Yang C N and Yang C P 1966 *Phys. Rev.* **150** 321–7
[12] Babelon O, de Vega H J and Viallet C 1983 *Nucl. Phys.* B **220** 13
[13] Grisaru M, Mezincescu L and Nepomechie R 1995 *J. Phys. A: Math. Gen.* **28** 1027