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

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### Abstract

We study boundary bound states using the Bethe ansatz formalism for the finite  $XXZ$  ( $\Delta > 1$ ) chain in a boundary magnetic field  $h$ . Boundary bound states are represented by the “boundary strings” similar to those described in [1]. We find that for certain values of  $h$  the ground state wave function contains boundary strings, and from this infer the existence of two “critical” fields in agreement with [2]. 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 the parallel fields. In the Ising ( $\Delta = \infty$ ) and isotropic ( $\Delta = 1$ ) limits our results agree with those previously known.

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One-dimensional 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, allowing basic physical properties to be extracted from the system of coupled transcendental equations. Among others, it allows 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 Letter we study the  $XXZ$  chain with even number of spins  $L$  in a boundary magnetic field,

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

in the regime  $\Delta > 1$ ,  $h_1 \geq 0$ ,  $h_2 \leq 0$ , focusing on the effects peculiar to systems with boundaries [6]. At  $h_1 = h_2 = 0$  this model describes one-dimensional antiferromagnet with non-magnetic impurities, accessible experimentally. We exploit the Bethe ansatz solution for this model, 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 sign of  $h$ ) boundary strings from the ground state wave-function. 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. This is not evident in the algebraic approach of [2].

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

$$E_{surf}(L, \Delta, h) = E_{gr} - E_{gr}^0, \quad (2)$$

in the thermodynamic limit  $L = \infty$ . Here  $E_{gr}$  is the ground state energy of (1) and  $E_{gr}^0$  is that of the periodic chain. We give an interpretation of our results in the limits  $\Delta \rightarrow \infty$  and  $\Delta \rightarrow 1$ , 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  $\Delta$ . 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 wave-function

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

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

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

The energy and spin of the  $n$ -magnon state are given by [7]:

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

It is convenient to rewrite BE using the following mappings:

$$\Delta = \cosh \gamma \geq 1, \quad \gamma \geq 0, \quad (6)$$

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

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

$$h = \cosh \gamma + \frac{\sinh \frac{\gamma}{2}(1-H)}{\sinh \frac{\gamma}{2}(1+H)} = \sinh \gamma \cdot \coth \frac{\gamma}{2}(H+1), \quad h_{lim} < |h| < \infty, \quad (8)$$

$$h = \cosh \gamma - \frac{\cosh \frac{\gamma}{2}(1-H)}{\cosh \frac{\gamma}{2}(1+H)} = \sinh \gamma \cdot \tanh \frac{\gamma}{2}(H+1), \quad |h| < h_{lim}. \quad (9)$$

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  $h_{lim} \equiv h(\infty) = \sinh \gamma$  lies between two critical fields  $h_{cr}^{(1)}, h_{cr}^{(2)}$  defined as follows [2] :

$$h_{cr}^{(1)} = \Delta - 1, \quad h_{cr}^{(2)} = \Delta + 1. \quad (10)$$

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

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

where

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

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

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

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

In the thermodynamic limit  $L \rightarrow \infty$  the real roots  $\alpha_j$  of BE form a dense distribution in the open interval  $(0, \pi)$  with density  $\rho(\alpha)$ ,  $dI = 2L(\rho + \rho^h)d\alpha$  being the number of roots in the interval  $d\alpha$ . The logarithm of eq. (11) is:

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

where  $I_j$  form an increasing sequence of positive integers, and

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

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

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

with

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

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 wave-function (3) vanish identically [5].

In eq. (17) the “boundary terms” are down by the 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

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

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

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

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

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

An elementary “bulk” excitation above the vacuum in the 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  $\theta$  can be easily computed:

$$\varepsilon_h(\theta) = \sinh \gamma \sum_{n=-\infty}^{\infty} \frac{(-1)^n e^{in\theta}}{\cosh \gamma n} > 0, \quad (22)$$

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

Analogous arguments can be applied to analyze “bulk” string solutions with complex  $\alpha$ . 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 discussed the bulk excitations, which are essentially the same as in the periodic chain. Let us now turn to the new solutions of eq. (11), boundary strings. The analysis is close to that of [1]. Boundary excitations have their wave-function (3) localized at  $x = 0$  or  $x = L$ , and in the limit  $L \rightarrow \infty$  the two boundaries may be considered separately. Let us study first the left boundary,  $h_1 > 0$ . The fundamental boundary 1-string consists of one root located at  $\alpha_0 = -i\gamma H_1$  for  $0 < h_1 < h_{cr}^{(1)}$ , and at  $\alpha_0 = \pi - i\gamma H_1$  for  $h_{cr}^{(2)} < h_1 < \infty$  (in both cases  $-1 < H_1 < 0$ ). It 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  $L \rightarrow \infty$  and  $\alpha \rightarrow \alpha_0$ . When  $h_{cr}^{(1)} < h_1 < h_{cr}^{(2)}$ , no such solution exists. Introduction of such a string into the vacuum whose root density  $\rho(\alpha)$  satisfies

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

leads to the redistribution of roots described by  $\delta\rho \equiv 2L(\tilde{\rho} - \rho)$ .  $\delta\rho$  is a solution of the equation

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

Solving (24), we find

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

For the energy and spin of the boundary 1-string with respect to the Dirac sea we obtain:

$$\tilde{\varepsilon}_b = -2 \sinh \gamma p'(\alpha_0) - \sinh \gamma \int_{-\pi}^{\pi} \delta\rho p'(\alpha) d\alpha = -\sinh \gamma \sum_{n=-\infty}^{\infty} \frac{(-1)^n e^{in\alpha_0}}{\cosh \gamma n}, \quad S_z = -1/2. \quad (26)$$

We see that the energy (26) is negative, so the correct ground state wave-function (3) should contain the boundary 1-string root  $\alpha_0$  when the value of  $h_1$  is not in the gap  $h_{cr}^{(1)} < h_1 < h_{cr}^{(2)}$ .

The ground state density  $\tilde{\rho}$  in this case satisfies the equation

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

The boundary excitation is obtained by removing from vacuum the root  $\alpha_0$ , which means that it has the energy  $-\tilde{\varepsilon}_b > 0$  and spin  $1/2$ , equal to the spin of the bulk elementary excitation. Substituting the value of  $\alpha_0$  into (26), we get the boundary excitation energy, which precisely agrees with the one obtained in [2]:

$$\varepsilon_b(h_1) = \sinh \gamma \sum_{n=-\infty}^{\infty} \frac{(-1)^{\kappa n} e^{\gamma H_1 n}}{\cosh \gamma n}, \quad -1 < H_1 < 0, \quad (28)$$

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

From (22) and (28) we see that for  $h_1 < h_{cr}^{(1)}$  the energy of the boundary excitation is smaller than the energy of the zero-rapidity bulk excitation, and becomes equal to it at  $h_1 = h_{cr}^{(1)}$ . So in this regime we may interpret the boundary excitation as the bound state of the kink, which gets unbound at  $h_1 = h_{cr}^{(1)}$ . For  $h_1 > h_{cr}^{(2)}$  such interpretation is impossible because the energy gap is smaller than the boundary excitation energy.

Besides the fundamental boundary 1-string, there exists an infinite set of “long” boundary strings, consisting of roots  $\alpha_0 - 2ik\gamma, \alpha_0 - 2i(k-1)\gamma, \dots, \alpha_0 + 2ni\gamma$  with  $n, k \geq 0$ . 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 “center of mass” has positive imaginary part and the lowest root  $\alpha_0 - 2ik\gamma$  lies below the real axis. Thus sufficiently long boundary string solutions exist even in the region  $h_{cr}^{(1)} < h_1 < h_{cr}^{(2)}$ . However, a direct calculation shows that their energy vanishes with respect to the vacuum, so they represent charged vacua.<sup>1</sup> (Analogous phenomenon occurs for the “long” strings in the bulk [12]: if the imaginary part of  $\alpha$  lies outside the strip  $-2\gamma < \text{Im}\alpha < 2\gamma$ , it gives no contribution to the energy.) For  $0 < h_1 < h_{cr}^{(1)}$  and  $h_{cr}^{(2)} < h_1 < \infty$  the  $(n,0)$  strings also represent charged vacua, while  $(n,k)$  strings with  $k \geq 1$  have the same energy (28) as the boundary bound state found above, and hence represent charged boundary excitations.<sup>2</sup>

Consider now the right boundary,  $h_2 < 0$  ( $H_2 < -1$ ). Now the fundamental boundary 1-string solution  $\alpha_0 = -i\gamma H_2$  exists for any value of  $h_2$  in the interval  $-h_{lim} < h_2 < 0$  (resp.  $\alpha_0 = \pi - i\gamma H_2$  for  $h_2 < -h_{lim}$ ). Explicit calculation shows that it has non-vanishing energy only if  $-2 < H_2 < -1$ , which corresponds to  $-h_{cr}^{(1)} < h_2 < 0$  (resp.  $h_2 < -h_{cr}^{(2)}$ ). For such values of  $h_2$  the energy of the 1-string with respect to the Dirac sea is positive and equal to  $\varepsilon_b(-h_2)$  (see eq. (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  $|h_{cr}^{(1)}|$  and

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<sup>1</sup>As an example, consider the boundary  $(1,0)$ -string consisting of the roots  $\alpha_0 + 2i\gamma, \alpha_0$ . 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.

<sup>2</sup>*E.g.*,  $(1,1)$  string with roots  $\alpha_0 + 2i\gamma, \alpha_0, \alpha_0 - 2i\gamma$  has  $S_z = -3/2$  and energy given by (28) with respect to the physical vacuum.



$|h_{cr}^{(2)}|$ , one with a 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 an integer (see (5)), we conclude that a boundary excitation can appear only 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, eq. (2), of the model (1), one should use eq. (14) in the limit  $L = \infty$  with the root density determined from eqs. (23) or (27) and the boundary terms (12) or (13), depending on the value of  $h$ . Define for convenience

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

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

1)  $|h_{1,2}| < h_{cr}^{(1)}$ . 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 eqs. (13),(18), and (27) and subtracting the bulk contribution (21) we get

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

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

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

3)  $h_{cr}^{(1)} < |h_{1,2}| < h_{lim}$ . The ground state has no boundary strings and its spin is zero.

From (23) and (13) one obtains the same expression as in case 1).

4)  $h_{lim} < |h_{1,2}| < h_{cr}^{(2)}$ . From (23) and (12) one obtains the same expression as in case 2).

The ground state has the same structure as in case 3).

A qualitative plot of the surface energy as a function of  $h$  ( $h = h_1 = -h_2$ ) is given in Fig.1. 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)-(9). In this sense the fields  $h_{cr}^{(1,2)}$  are not actually “critical.” We find for  $h_1 = h_2 = 0$  the value

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

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

$$\mathcal{H} = \frac{1}{2} \left\{ \sum_{i=1}^{L-1} \Delta \sigma_i^z \sigma_{i+1}^z + h_1 \sigma_1^z + h_2 \sigma_L^z \right\}, \quad (33)$$

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

$$h \approx \Delta \pm e^{-\gamma H}, \quad (34)$$

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 independent of  $\theta$  and equal to  $\Delta$ , since only  $n = 0$  term contributes to the sum. The energy of the boundary bound state (28) becomes  $\varepsilon_b = \Delta \pm e^{-\gamma H} = h$ . This suggests the following interpretation in terms of the Ising chain: in the Ising ground state the  $i$ -th spin has the value  $(-1)^i$ . Local bulk excitation of the smallest energy  $2\Delta$  can be obtained by flipping one spin (the first spin excepted). The arising two surfaces (domain walls) separating the flipped spin from its right and left neighbours are called kinks and carry the energy  $\Delta$  each. The kink corresponds to a hole

in the Dirac sea in the Bethe ansatz picture, and these holes can exist only in pairs, which is obviously the case for the kinks in the Ising chain. 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 1 excitation, one has charge 0 excitation of the same energy obtained by flipping any even number of spins in a row. In the BA this corresponds to the “2 holes and 2-string” state. The boundary bound state is obtained by flipping the first (or the last) spin. Such a state has the energy  $h_1 + \Delta$  above the vacuum energy in the Ising limit, where  $h_1$  is the contribution of the boundary term in eq. (33) and  $\Delta$  is the energy of the kink created because of the interaction of the boundary spin with the bulk ones. 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 ground state 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  $\gamma \rightarrow \infty$  in eqs. (30)-(31), we obtain the expected result  $E_{surf} \rightarrow (\Delta - h_1 + h_2)/2$ .

In the isotropic (rational) limit  $\Delta \rightarrow 1$  (*i.e.*,  $\gamma \rightarrow 0$ ) one gets the XXX chain in a boundary magnetic field, which was discussed in the BA framework in [13] for  $0 < h_1, h_2 < 2$ . From (8)-(9) one has in this limit

$$h = \frac{2}{1 + H}. \quad (35)$$

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

$$E_{surf} = \frac{1}{2}(h_1 + h_2) - \frac{1}{2} + \frac{\pi}{2} - \int_0^\infty dx \frac{e^{-(\frac{2}{h_1}-1)x} - e^{(\frac{2}{h_2}-1)x} + e^{-x}}{\cosh x}$$

$$= \frac{1}{2}(h_1 - h_2) - \frac{1}{2} + \frac{\pi}{2} - \int_0^\infty dx \frac{e^{-(\frac{2}{h_1}-1)x} + e^{(\frac{2}{h_2}+1)x} + e^{-x}}{\cosh x}, \quad (36)$$

where the second line was obtained from the first one after a simple manipulation. We can compare this result with that of [13] and find the agreement. For  $h_1 = h_2 = 0$  one has from (36):  $E_{surf} = (\pi - 1)/2 - \ln 2$ .

Another aspect is the structure of the ground state in the regime  $h_{1,2} > 0$ . Assuming that, for example, for  $h_{1,2} > h_{cr}^{(2)}$  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 of 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  $\gamma \rightarrow \infty$ , 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 called a boundary excitation at one of the ends. This suggests that for finite  $\Delta$  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  $h_{1,2} > h_{cr}^{(2)}$ . Such a state has spin zero. Since the energy difference between this ground state and a state with a moving (instead of stationary) kink vanishes when the rapidity of the kink goes to zero, the spectrum acquires a gapless branch.<sup>3</sup> Similarly, when  $h_{cr}^{(1)} < h_{1,2} < h_{cr}^{(2)}$ , for the ground state to have the integer charge, it should also contain a kink in the bulk. When  $h_{1,2} < h_{cr}^{(1)}$  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 to have either left or right boundary

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<sup>3</sup>In the Ising limit  $\gamma \rightarrow \infty$  the energy of the kink is independent of rapidity, and therefore this branch degenerates to the vacuum.

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  $h_{1,2} < h_{cr}^{(1)}$  than the one with a hole in the bulk and two boundary strings, while for  $h_{1,2} > h_{cr}^{(2)}$  the state with the bulk hole is energetically preferable, since in this case  $\varepsilon_b > \varepsilon_h$  (see Fig.2 and [2]). This situation is in some sense analogous to the case of the periodic  $XXZ$  chain with odd  $L$ , where the ground state contains a kink. Let us mention that according to the above discussion the surface energy in the case  $h_{1,2} > h_{lim}$  is:

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

In the rational ( $\gamma \rightarrow 0$ ) limit  $\varepsilon_h(0)$  vanishes and eq. (37) becomes

$$E_{surf} = \frac{1}{2}(h_1 + h_2) - \frac{1}{2} + \frac{\pi}{2} - \int_0^{\infty} dx \frac{e^{-(\frac{2}{h_1}-1)x} + e^{-(\frac{2}{h_2}-1)x} + e^{-x}}{\cosh x}. \quad (38)$$

This expression agrees with the one obtained in [13]. Note that the authors of [13] obtained eq. (38) under assumption that  $0 < h_{1,2} < h_{cr}$ , while our derivation shows that this result is valid for  $0 < h_{1,2} < \infty$ . In the Ising limit eq. (37) gives the correct result  $E_{surf} = (3\Delta - h_1 - h_2)/2$ .

In conclusion we would like to mention that within the BA technique it is possible to calculate also 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] by the algebraic approach.

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FIGURES

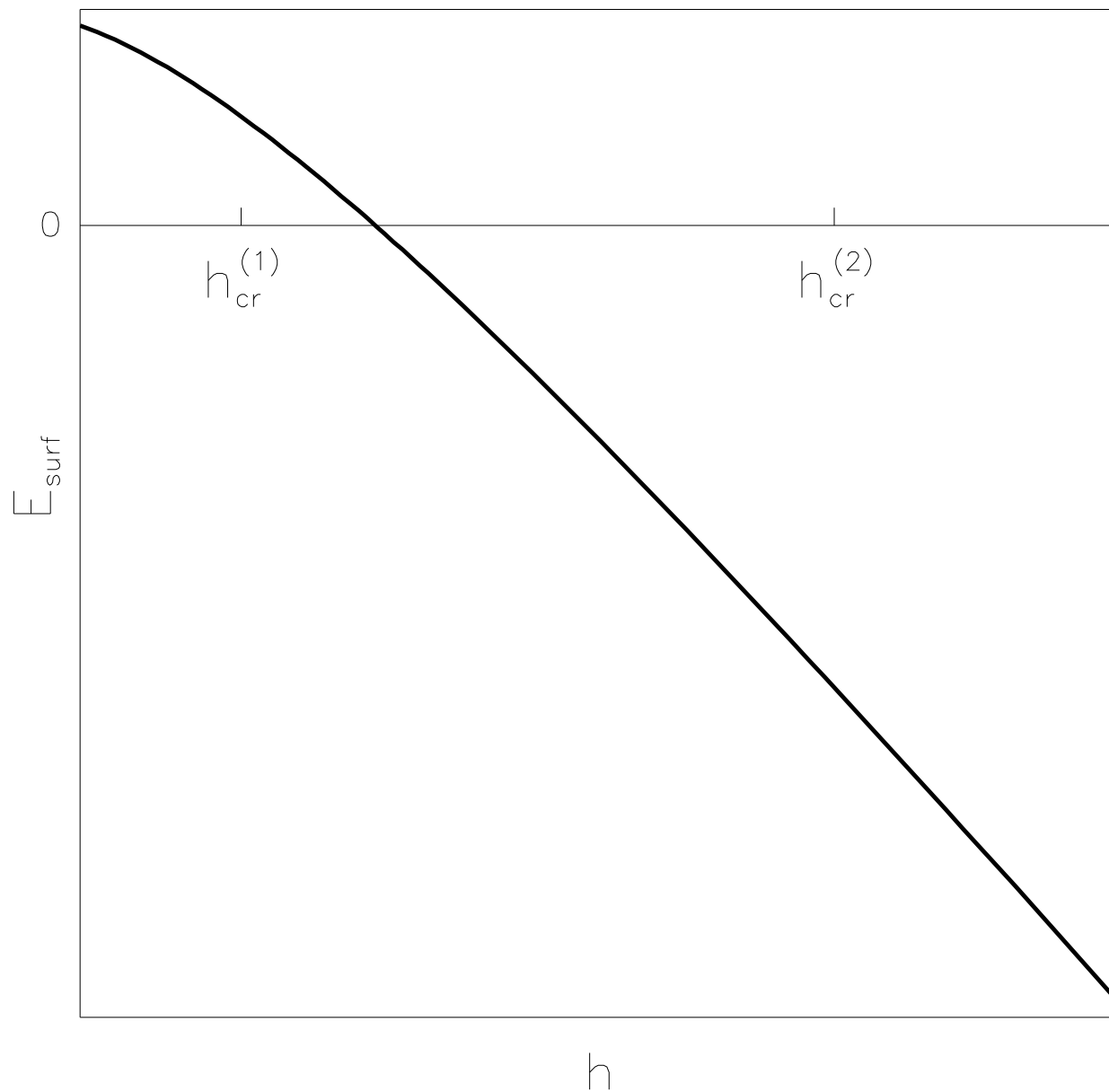


FIG. 1. A schematic plot of the ground state surface energy as a function of the boundary magnetic field  $h = h_1 = -h_2$ . The critical fields are also shown.

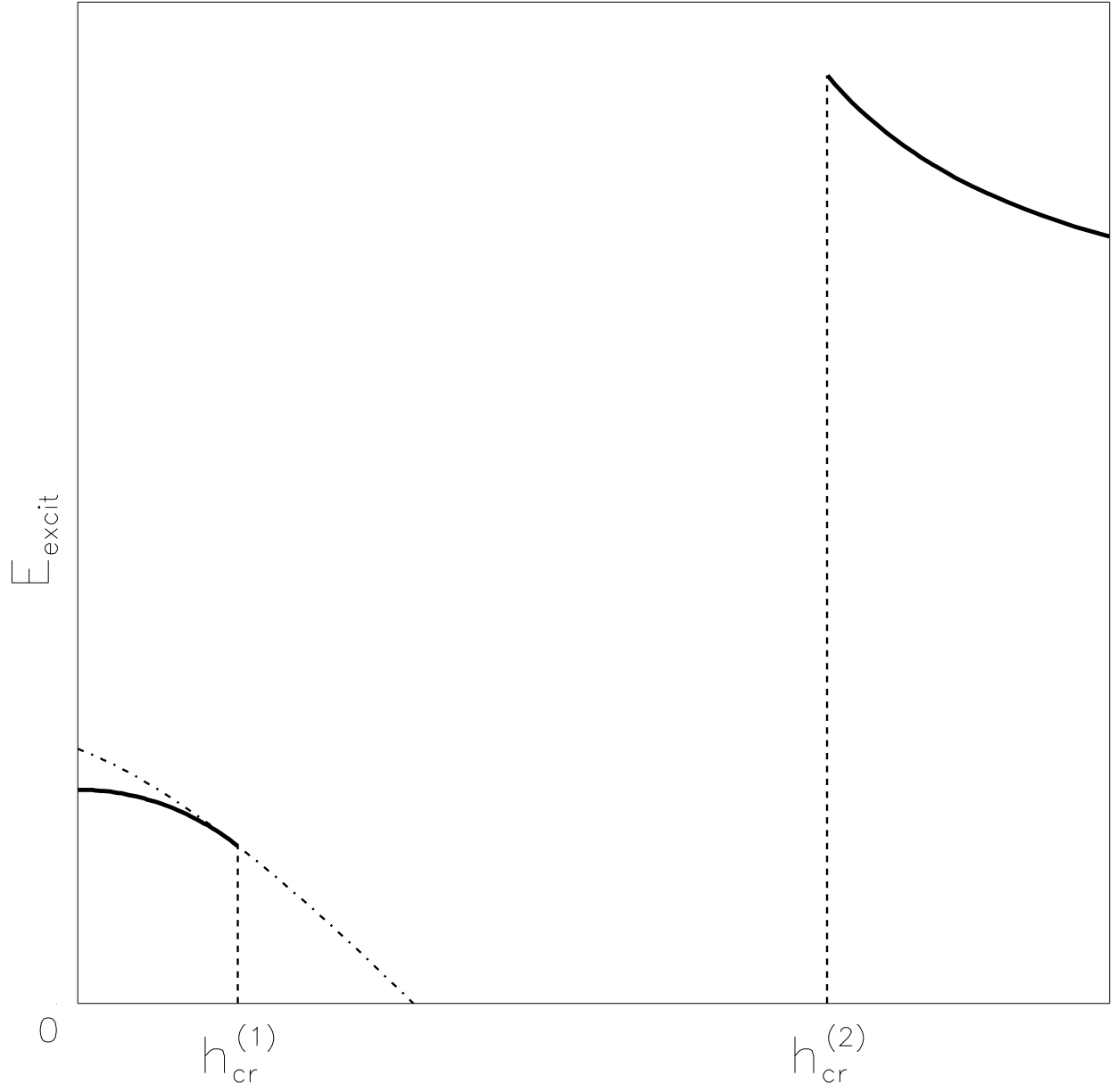


FIG. 2. Solid line: a schematic plot of the surface energy of the state with a boundary excitation at one of the ends,  $E_{surf}(h) + \varepsilon_b(h)$ , as a function of the boundary magnetic field  $h = h_1 = -h_2$ . Dash-dotted line: the energy of the state containing a zero rapidity hole in the bulk  $E_{surf}(h) + \varepsilon_h(0)$ .