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## The XX model with boundaries: II. Finite-size scaling and partition functions

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**Abstract.** We compute the continuum limit of the spectra for the XX model with arbitrary complex boundary fields. In the case of Hermitian boundary terms one obtains the partition functions of the free compactified boson field on a cylinder with Neumann–Neumann, Dirichlet–Neumann or Dirichlet–Dirichlet boundary conditions. This also applies for certain non-Hermitian boundaries. For special cases we also compute the free surface energy. For certain non-Hermitian boundary terms the results are more complex. Here one obtains logarithmic corrections to the free surface energy. The asymmetric version of the XX model with boundaries (this includes the Dzyaloshinsky–Moriya interaction) is also discussed.

### 1. Introduction

In the first paper of this series [1] we showed how to diagonalize the Hamiltonian of the XX model with boundaries

$$H = \frac{1}{2} \sum_{j=1}^{L-1} [\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+] + \frac{1}{\sqrt{8}} [\alpha_- \sigma_1^- + \alpha_+ \sigma_1^+ + \alpha_z \sigma_1^z + \beta_+ \sigma_L^+ + \beta_- \sigma_L^- + \beta_z \sigma_L^z] \quad (1)$$

by introducing an auxiliary Hamiltonian

$$H_{\text{long}} = \frac{1}{2} \sum_{j=1}^{L-1} [\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+] + \frac{1}{\sqrt{8}} [\alpha_- \sigma_0^x \sigma_1^- + \alpha_+ \sigma_0^x \sigma_1^+ + \alpha_z \sigma_1^z + \beta_+ \sigma_L^+ \sigma_{L+1}^x + \beta_- \sigma_L^- \sigma_{L+1}^x + \beta_z \sigma_L^z] \quad (2)$$

which in turn may be diagonalized in terms of free fermions. The parameters  $\alpha_{\pm}$ ,  $\beta_{\pm}$ ,  $\alpha_z$  and  $\beta_z$  are arbitrary complex numbers. Note that  $H_{\text{long}}$  commutes with  $\sigma_0^x$  and  $\sigma_{L+1}^x$ . Hence the spectrum of  $H_{\text{long}}$  decomposes into four sectors (+, +), (+, −), (−, −), (−, +) corresponding to the eigenvalues  $\pm 1$  of  $\sigma_0^x$  and  $\sigma_{L+1}^x$ . The spectrum of  $H$  is obtained by projecting onto the (+, +) sector.

While in [1] our focus was on the diagonalization of the finite chain, here we are going to examine the asymptotic behaviour of the energy levels for large values of  $L$ . In the case of conformal invariance this information is usually encoded in the partition function, which we define by

$$\mathcal{Z} = \lim_{L \rightarrow \infty} \text{tr} z^{(L/\xi)(H - e_{\infty} L - f_{\infty})} \quad (3)$$

where  $z < 1$  and  $e_\infty$  and  $f_\infty$  denote the free bulk and the free surface energy, respectively.  $\xi$  may be considered as a normalization constant here. We will also consider the partition function for  $H_{\text{long}}$ .

In the case of periodic boundary conditions the continuum limit of the XXZ chain can be described by a free boson field  $\Phi$  (see, e.g., [2]), with action

$$S = \frac{1}{2} \int dx_1 dx_2 [(\partial_1 \Phi)^2 + (\partial_2 \Phi)^2] \quad (4)$$

being compactified on a circle of radius  $r$ , i.e. we identify  $\Phi$  with  $\Phi + 2\pi r$  (we follow the notation of [3]). The radius of compactification  $r$  is related to the value of the anisotropy in the XXZ model. At the free fermion point the anisotropy is zero and we have  $r = 1/\sqrt{4\pi}$ .

Consider the boson field on a cylinder of length  $L$  and circumference  $N$  imposing periodic boundary conditions in the direction of the cylinder's length. Quantizing the field with time in  $N$ -direction yields the partition function [3]

$$\mathcal{Z}_{\text{periodic}} = \frac{1}{\eta(q)^2} \sum_{m,n \in \mathbb{Z}} q^{\frac{1}{2}(m^2/2\pi r^2 + 2\pi r^2 n^2)} \quad (5)$$

where  $q = e^{-2\pi N/L}$  and

$$\eta(q) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n). \quad (6)$$

This expression coincides with the partition function for the periodic XXZ chain, which has been studied extensively in [4–6]. The partition function for  $H_{\text{long}}$  in the periodic case is just  $4\mathcal{Z}_{\text{periodic}}$ .

Now consider the case of open boundaries at both ends of the cylinder. There are two different boundary conditions preserving conformal invariance, i.e. the Dirichlet and the Neumann boundary conditions (see, e.g., [3, 7]). This yields three different partition functions corresponding to the various possible combinations of the two boundary conditions. The respective partition functions can be found in [3, 7]. Imposing Dirichlet boundary conditions at both ends of the cylinder results in

$$\mathcal{Z}_{\text{DD}}(\Delta) = \frac{1}{\eta(q)} \sum_{n \in \mathbb{Z}} q^{\frac{1}{2}(2\sqrt{\pi}rn + \Delta)^2} \quad (7)$$

where  $q = e^{-\pi N/L}$  and  $\Delta = (\Phi_0 - \Phi_L)/\sqrt{\pi}$ . We denote the values of the boson field at the boundaries by  $\Phi_0$  and  $\Phi_L$ . This type of partition function has also been obtained for the open XXZ chain with diagonal, Hermitian boundary fields [8].

The Neumann–Neumann partition function is given by

$$\mathcal{Z}_{\text{NN}}(\Delta) = \frac{1}{\eta(q)} \sum_{m \in \mathbb{Z}} q^{2(m/(2\sqrt{\pi}r) + \Delta/2)^2} \quad (8)$$

where  $\Delta = (\tilde{\Phi}_0 - \tilde{\Phi}_L)/\sqrt{\pi}$  and  $\tilde{\Phi}_0, \tilde{\Phi}_L$  denote the values of the dual field  $\tilde{\Phi}$  at the boundaries [3, 7]. The Dirichlet–Neumann boundary condition yields [3, 7]

$$\mathcal{Z}_{\text{DN}} = \frac{1}{2\eta(q)} \sum_{k \in \mathbb{Z}} q^{\frac{1}{4}(k - \frac{1}{2})^2}. \quad (9)$$

In this case no free parameter appears.

Which boundary conditions of the Hamiltonian  $H$  lead to the partition functions (8) and (9) is not yet known. We will close this gap. We are going to see that, as long as the Hamiltonian

$H$  is Hermitian, the partition function of the chain corresponds to one of the three boson partition functions for open boundaries. However, this may also be the case for certain non-Hermitian boundary terms. See section 2 for a survey over the boundary conditions which we will consider.

In [9] it has been argued that non-diagonal boundary terms correspond to Neumann boundary conditions for the boson field. Our results will show that this assumption is correct in the Hermitian case, but not necessarily for non-Hermitian boundaries.

In this paper we also study the asymmetric XX chain with boundaries (see equation (25)). This includes the quantum chain with Dzyaloshinsky–Moriya interactions, which was already studied in [10] for free and toroidal boundary conditions. The partition function for real values of  $p$  and  $q$  in (25) and periodic boundary conditions was obtained in [13]. The special case  $p = 1$  and  $q = 0$  with boundaries has already been studied in [11].

This paper is organized as follows. We will start with a summary of our results for the symmetric chain with Hermitian and non-Hermitian boundaries in section 2. The asymmetric XX chain will be discussed in section 3. We will give our conclusions in section 4. The appendix is dedicated to the computation of the fermion energies which yield the energy gaps of the chain.

## 2. Summary of results

The structure of our results is most simply encoded in terms of new parameters  $F, C, G, K, J$ , where

$$\begin{aligned}
 F &= 4\alpha_- \alpha_+ \beta_+ \beta_- \\
 C &= \alpha_-^2 \beta_+^2 + \alpha_+^2 \beta_-^2 \\
 G &= 2\alpha_- \alpha_+ (1 + 2\beta_z^2) + 2\beta_- \beta_+ (1 + 2\alpha_z^2) \\
 K &= 2(\alpha_- \alpha_+ + \beta_- \beta_+) + (1 + 2\alpha_z^2)(1 + 2\beta_z^2) \\
 J &= 8\alpha_z \beta_z - 4\alpha_z^2 \beta_z^2 + 2(\alpha_- \alpha_+ + \beta_- \beta_+) + 2\alpha_z^2 + 2\beta_z^2 - 1.
 \end{aligned}
 \tag{10}$$

The six different situations we considered are given in table 1. This table also indicates which kind of partition function we obtained for  $H$ . For Hermitian boundaries the cases in this table cover the whole parameter space. This is not the case for non-Hermitian boundary terms.

For the cases in table 1 we computed analytically the energy gaps in the leading order as shown in the appendix. The exact ground-state energies for certain cases listed in table 2 have already been obtained in [1].

**Table 1.** Conditions on the parameters  $F, C, G, K, J$  considered in this paper. An asterisk indicates that the corresponding value may be arbitrary. The partition functions  $\mathcal{Z}_{DD}, \mathcal{Z}_{NN}$  and  $\mathcal{Z}_{DN}$  are defined in (7)–(9). For the last two cases we obtained anomalous behaviour of the energies (see section 2.5). We use ‘h’ and ‘n-h’ as abbreviations for Hermitian and non-Hermitian, respectively.

F	C	G	K	J		
$\neq 0$	*	*	*	*	$\mathcal{Z}_{NN}$	h and n-h
0	0	$\neq 0$	*	*	$\mathcal{Z}_{DN}$	h and n-h
0	0	0	$\neq 0$	*	$\mathcal{Z}_{DD}$	h and n-h
0	0	0	0	0	$2 \times \mathcal{Z}_{DD}$	n-h
0	$\neq 0$	$\neq 0$	*	*	Anom.	n-h
0	0	0	0	$\neq 0$	Anom.	n-h

**Table 2.** The values of the parameters  $F, C, G, K, J$  for the cases where the ground-state energy of  $H_{\text{long}}$  has been obtained in [1]. The table shows the free surface energy  $f_\infty$  and the lowest highest weight  $h_{\text{min}}$  (cf (11)). The expressions for  $f_\infty$  are also valid for  $H$ .  $\zeta$  denotes a free parameter, which has to be chosen such that  $0 \leq \text{Re } \zeta \leq 2\pi$  for case 12 and  $-\pi < \text{Re } \zeta < \pi$  otherwise.

Case	$F$	$(-1)^L C$	$G$	$H$	$J$	$f_\infty$	$h_{\text{min}}$	
							$L$ even	$L$ odd
1	2	0	5	4	2	$\frac{1}{4} - 3/2\pi$	$\frac{1}{32}$	$\frac{1}{32}$
2	0	0	2	3	1	$\frac{1}{4} - 4/\pi$	$\frac{1}{16}$	$\frac{1}{16}$
3	0	0	1	2	0	$\frac{1}{2} - 3/2\pi$	$\frac{1}{16}$	$\frac{1}{16}$
4	0	0	4	4	2	$-1/2\pi$	$\frac{1}{16}$	$\frac{1}{16}$
5	1	$\frac{1}{2}$	3	3	1	$\frac{1}{2} - 2/\pi$	0	$\frac{1}{8}$
6	1	$-\frac{1}{2}$	3	3	1	$\frac{1}{2} - 2/\pi$	$\frac{1}{8}$	0
7	2	1	5	4	2	$\frac{1}{4} - 3/2\pi$	0	$\frac{1}{8}$
8	2	-1	5	4	2	$\frac{1}{4} - 3/2\pi$	$\frac{1}{8}$	0
9	4	$(-1)^L 2 \cos \zeta$	8	5	3	$-1/\pi$	$\frac{\zeta^2}{(8\pi^2)}$	$\frac{\zeta^2}{(8\pi^2)}$
10	$2 + 2 \cos \zeta$	$1 + \cos \zeta$	$4 + 4 \cos \zeta$	$3 + 2 \cos \zeta$	$1 + \cos \zeta$	$\frac{1}{2} - 1/\pi - \frac{1}{2} \cos \frac{1}{2} \zeta$	0	$\frac{1}{8}$
11	$4 + 4 \cos \zeta$	0	$6 + 6 \cos \zeta$	$4 + 2 \cos \zeta$	$2 + 2 \cos \zeta$	$\frac{1}{4} - 1/2\pi - \frac{1}{2} \cos \frac{1}{2} \zeta$	$\frac{1}{32}$	$\frac{1}{32}$
12	$2 - 2 \cos \zeta$	$\cos \zeta - 1$	$2 - 2 \cos \zeta$	4	4	$\frac{1}{2} - \frac{1}{2} (\cos \frac{1}{4} \zeta + \sin \frac{1}{4} \zeta)$	$\frac{1}{8}$	0
13	$4 + 4 \cos \zeta$	$-2 - 2 \cos \zeta$	$4 + 4 \cos \zeta$	$4 + 2 \cos \zeta$	$4 + 2 \cos \zeta$	$\frac{1}{2} - 1/(2\sqrt{2}) - \frac{1}{2} \cos \frac{1}{2} \zeta$	$\frac{1}{8}$	0
14	$8 + 8 \cos \zeta$	$-2 - 2 \cos \zeta$	$8 + 8 \cos \zeta$	$6 + 2 \cos \zeta$	$2 \cos \zeta - 2$	$-\frac{1}{2} \cos \frac{1}{2} \zeta$	0	$\frac{1}{8}$
15	$8 + 8 \cos \zeta$	$-4 - 4 \cos \zeta$	$6 + 6 \cos \zeta$	$6 + 2 \cos \zeta$	$6 + 2 \cos \zeta$	$-\frac{1}{2} \cos \frac{1}{2} \zeta$	$\frac{1}{8}$	0
16	0	0	0	$2 + 2 \cos \zeta$	$2 + 2 \cos \zeta$	$\frac{1}{2} - \frac{1}{2} \cos \frac{1}{2} \zeta$	$\frac{1}{8}$	0

However, the information of the energy gaps is already sufficient to obtain the partition functions for  $H_{\text{long}}$  up to a factor of  $z^{-\frac{1}{24} + h_{\text{min}}}$ , where  $h_{\text{min}}$  denotes the lowest highest weight appearing in the representation of the Virasoro algebra. This information has to be extracted from the ground-state energies [12],

$$E_0 = e_\infty L + f_\infty - \frac{\pi}{L} \left( \frac{1}{24} - h_{\text{min}} \right) + \dots \tag{11}$$

The value of the free bulk energy is already known from the periodic chain, i.e.  $e_\infty = -1/\pi$  [14]. The values of the free surface energies  $f_\infty$  and of  $h_{\text{min}}$  have been obtained for the cases given in table 2 expanding the exact expressions for the finite chain given in [1].

The results confirm the partition functions we will give for  $H_{\text{long}}$  in the following. For the cases not listed in table 2 we checked our expressions numerically. The partition functions for  $H$  have been obtained afterwards by projecting onto the  $(+, +)$ -sector (see [1] for details on the projection mechanism). We are now going to discuss the cases given in table 1 in detail.

### 2.1. Neumann–Neumann boundary conditions

The condition  $F \neq 0$  simply implies that all non-diagonal boundary terms are present. The diagonal terms may be arbitrary. It is quite instructive to introduce a new parametrization of the boundary parameters  $\alpha_\pm$  and  $\beta_\pm$  as follows:

$$\begin{aligned} \alpha_+ &= R_\alpha e^{i\pi\varphi} & \alpha_- &= R_\alpha e^{-i\pi\varphi} \\ \beta_+ &= R_\beta e^{i\pi(\chi+\varphi)} & \beta_- &= R_\beta e^{-i\pi(\chi+\varphi)} \end{aligned} \tag{12}$$

where  $R_\alpha, R_\beta \in \mathbb{R}^+, \chi, \varphi \in \mathbb{R}, -1 < \chi \leq 1$ . The value of  $\Delta$  which enters the partition function (8) is then given by

$$\Delta = \begin{cases} \chi & \text{for } L \text{ odd} \\ \chi + 1 & \text{for } L \text{ even.} \end{cases} \tag{13}$$

The partition function for  $H_{\text{long}}$  is given by

$$\mathcal{Z}_{\text{long}} = 2\mathcal{Z}_{\text{NN}}(\chi) + 2\mathcal{Z}_{\text{NN}}(\chi + 1) \tag{14}$$

for even and odd values of  $L$ . Note that the parametrization (12) does not work for non-Hermitian boundaries. In this case we may define the parameter  $\chi$  via

$$\chi = \frac{i}{2\pi} \ln \left( \frac{\alpha_- \beta_+}{\alpha_+ \beta_-} \right) \tag{15}$$

where the logarithm is taken in a way such that  $0 \leq |\text{Re}(\chi)| \leq \frac{1}{2}$  for  $\text{Re}(\alpha_+ \beta_- + \alpha_- \beta_+) > 0$  and  $1 \geq |\text{Re}(\chi)| \geq \frac{1}{2}$  for  $\text{Re}(\alpha_+ \beta_- + \alpha_- \beta_+) < 0$ . This rule is consistent with the parametrization (12), which implies  $\text{Re}(\alpha_+ \beta_- + \alpha_- \beta_+) = 2R_\alpha R_\beta \cos(\chi\pi)$ . However, we cannot perform the projection onto the  $(+, +)$ -sector in general if the boundaries are non-Hermitian. In this case our result for the partition function of  $H$  is restricted to the cases listed in table 2 which satisfy the conditions  $\alpha_z = \beta_z = 0$  or  $\alpha_+ = \alpha_-, \beta_+ = \beta_-$  [1]. The result for  $H_{\text{long}}$  is valid in general.

### 2.2. Dirichlet–Neumann boundary conditions

The conditions for the Dirichlet–Neumann case yield

$$\beta_\pm = 0 \quad \alpha_\pm \neq 0 \quad \beta_z \neq \pm \frac{i}{\sqrt{2}} \tag{16a}$$

or

$$\beta_\pm \neq 0 \quad \alpha_\pm = 0 \quad \alpha_z \neq \pm \frac{i}{\sqrt{2}}. \tag{16b}$$

The value of  $\alpha_z$ , respectively, of  $\beta_z$  may be arbitrary. The partition function for  $H_{\text{long}}$  is just  $\mathcal{Z}_{\text{long}} = 4\mathcal{Z}_{\text{DN}}$  for  $L$  even and odd. The case of one non-diagonal boundary at the end of a semi-infinite XX chain has already been considered in [15]. The author has shown that the model can be decoupled into two Ising models with different boundary conditions. One of them is subject to a free boundary condition at the end and the other one is subject to the fixed boundary condition. The partition functions for the Ising model with free and mixed boundary conditions are well known [12, 16]. Taking the product of them also results in (9).

### 2.3. Dirichlet–Dirichlet boundary conditions

The Dirichlet–Dirichlet partition function is obtained for two different types of boundary terms.

The first type is given by

$$\beta_z \neq \pm \frac{i}{\sqrt{2}} \quad \alpha_z \neq \pm \frac{i}{\sqrt{2}} \quad \beta_- = \alpha_- = 0 \tag{17}$$

where instead of the last equation we might have also chosen  $\beta_+ = \alpha_+ = 0$ . However, for this type of boundary the non-diagonal boundary terms have no influence on the energies even on the finite chain. The second type is given by

$$\beta_\pm = 0 \quad \alpha_\pm \neq 0 \quad \beta_z = \pm \frac{i}{\sqrt{2}} \tag{18a}$$

or

$$\beta_{\pm} \neq 0 \quad \alpha_{\pm} = 0 \quad \alpha_z = \pm \frac{i}{\sqrt{2}} \tag{18b}$$

where the values of  $\alpha_z$ , respectively,  $\beta_z$  may be chosen arbitrarily. Note that for this second type the boundary terms are non-Hermitian. For both types of boundaries the value of  $\Delta$  which enters (7) is given by

$$\Delta = \frac{1}{2\pi} \arccos \left( (-1)^{L+1} \frac{J}{K} \right). \tag{19}$$

The partition function for  $H_{\text{long}}$  is  $\mathcal{Z}_{\text{long}} = 4\mathcal{Z}_{\text{DD}}(\Delta)$  for even and odd  $L$ .

#### 2.4. $F = C = G = K = J = 0$

For the case  $F = C = G = K = J = 0$  the boundary parameters are nearly fixed, i.e.

$$\alpha_z = \pm \frac{i}{\sqrt{2}} \quad \beta_z = \mp \frac{i}{\sqrt{2}} \tag{20}$$

and  $\alpha_+ = \beta_+ = 0$  or  $\alpha_- = \beta_- = 0$ . This case is special. The partition function we obtained does not fit into the picture suggested by the analogy to the free boson. Here an additional zero mode appears. The value of  $\Delta$  is given by  $\Delta = 0$  for odd  $L$  and by  $\Delta = \frac{1}{2}$  for even  $L$ . The partition function for  $H_{\text{long}}$  is  $\mathcal{Z}_{\text{long}} = 8\mathcal{Z}_{\text{DD}}(\Delta)$  for  $L$  even and  $L$  odd.

#### 2.5. Anomalous behaviour

For the last two cases in table 1 we obtained logarithmic corrections to the free surface energy. Note that there is no case in table 2 which corresponds to the boundaries in question. However, we computed the ground-state energy  $E_0$  of  $H_{\text{long}}$  numerically for one example of boundaries which lead to the anomalous behaviour. Our computations suggest

$$E_0 \sim -\frac{L}{\pi} + f_{\infty} + \frac{1}{L} (\rho_1 \ln L + \rho_2) \tag{21}$$

where  $\rho_1$  and  $\rho_2$  are complex numbers. Figures 1 and 2 show the real, respectively, the imaginary part of the Casimir amplitude. The computation has been done for  $\alpha_z = 1/\sqrt{2}$ ,  $\beta_z = i/\sqrt{2}$ ,  $\alpha_{\pm} = \beta_{\pm} = 0$  which corresponds to the last case in table 1. In both cases the fermionic energies scale as

$$2\Lambda \sim \frac{1}{L} \left[ k\pi \pm \frac{1}{2} (\arg \Delta - i \ln L) \right] \quad k = 0, 1, 2, \dots \tag{22}$$

where the value of  $\Delta$  is given by

$$\Delta = -\frac{4C}{G} \tag{23}$$

for  $F = 0$ ,  $C, G \neq 0$ , respectively, by

$$\Delta = (-1)^L \frac{2J}{1 - 4\alpha_z^2 \beta_z^2} \tag{24}$$

for  $F = C = G = K = 0, J \neq 0$ . Our result for the last case only makes sense for  $(\alpha_z \beta_z)^2 \neq \frac{1}{4}$ . The factor of two in (22) is just a remnant from our notation in [1]. Note the integer spacing of the energy gaps (22).

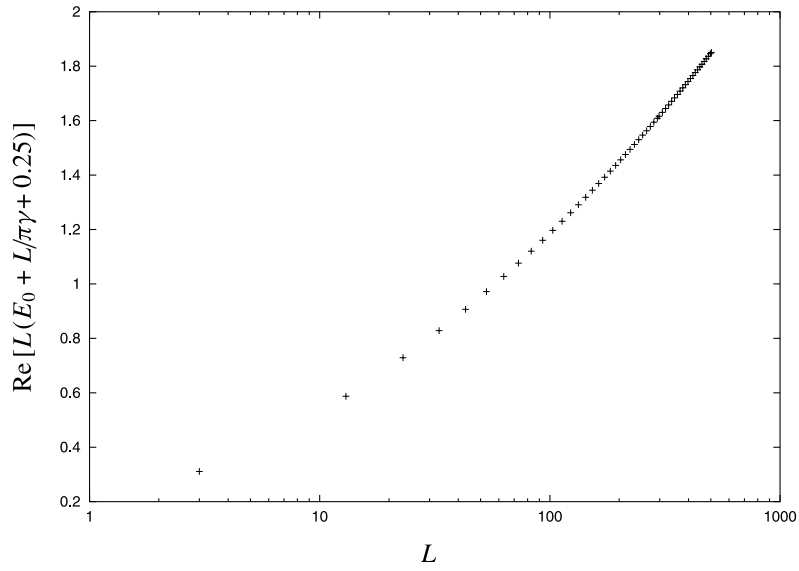


Figure 1. Real part of the Casimir amplitude ( $\alpha_z = 1/\sqrt{2}$ ,  $\beta_z = i/\sqrt{2}$ ,  $\alpha_{\pm} = \beta_{\pm} = 0$ ).

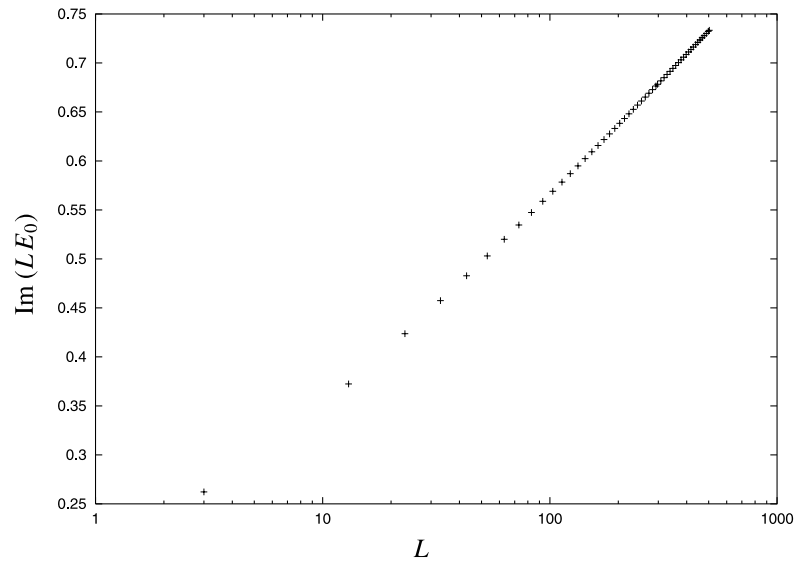


Figure 2. Imaginary part of the Casimir amplitude ( $\alpha_z = 1/\sqrt{2}$ ,  $\beta_z = i/\sqrt{2}$ ,  $\alpha_{\pm} = \beta_{\pm} = 0$ ).

### 3. The asymmetric XX chain

We also considered the asymmetric XX chain which is defined by the Hamiltonian

$$H_a = \sum_{j=1}^{L-1} [p\sigma_j^+ \sigma_{j+1}^- + q\sigma_j^- \sigma_{j+1}^+] + \frac{1}{\sqrt{8}} [\alpha'_- \sigma_1^- + \alpha'_+ \sigma_1^+ + \alpha_z \sigma_1^z + \beta'_- \sigma_L^- + \beta'_+ \sigma_L^+ + \beta_z \sigma_L^z]. \quad (25)$$



Without loss of generality we restrict ourselves to  $\sqrt{pq} = \frac{1}{2}$ . Under this condition  $H_a$  can be mapped on the symmetric chain (1) with boundary parameters

$$\begin{aligned} \alpha_- &= Q^{(1-L)/2} \alpha'_- & \alpha_+ &= Q^{(L-1)/2} \alpha'_+ \\ \beta_- &= Q^{(L-1)/2} \beta'_- & \beta_+ &= Q^{(1-L)/2} \beta'_+ \end{aligned} \tag{26}$$

by a similarity transformation, where  $Q = \sqrt{q/p}$ . The diagonal terms remain unchanged. We will separate two cases in the following. First we will consider Hermitian bulk terms, i.e.

$$p = e^{i\pi\kappa}/2 \quad q = e^{-i\pi\kappa}/2. \tag{27}$$

This corresponds to Dzyaloshinsky–Moriya-type interactions in the bulk. Thereafter we will turn to non-Hermitian bulk terms with  $p, q$  in  $\mathbb{R}$ .

### 3.1. Dzyaloshinsky–Moriya interactions

We restricted ourselves to Hermitian boundaries. In this case the value of  $\kappa$  only has an effect on the spectra if non-diagonal boundary terms are present at both ends of the chain. We introduce the parametrization

$$\begin{aligned} \alpha'_+ &= R'_\alpha e^{i\pi\varphi'} & \alpha'_- &= R'_\alpha e^{-i\pi\varphi'} \\ \beta'_+ &= R'_\beta e^{i\pi(\chi'+\varphi')} & \beta'_- &= R'_\beta e^{-i\pi(\chi'+\varphi')}. \end{aligned} \tag{28}$$

According to (26) and (12) the mapping onto symmetric bulk terms yields

$$R'_\alpha = R_\alpha \quad R'_\beta = R_\beta \quad \varphi = \varphi' + \frac{1}{2}\kappa(1 - L) \quad \chi = \chi' + \kappa(L - 1) \bmod 2. \tag{29}$$

Remember that in the case of length-independent boundary terms, the value of  $\chi$  contains the full information about the partition function. Observe now, that it is possible to choose values of  $\kappa$  such that the value of  $\chi$  in (29) becomes independent of  $L$  as long as one considers only certain sequences of lattice lengths. This is exactly the case if  $\kappa/2$  is rational, i.e.  $\kappa/2 = m/n, m \in \mathbb{Z}, n \in \mathbb{N}^+$ . In this case  $\chi$  is independent of  $L$  for  $L = ln + r, 0 \leq r < n, l \in \mathbb{N}$ , i.e.

$$\chi = \chi' + \frac{2m(r - 1)}{n}. \tag{30}$$

The results obtained for the symmetric case can be adopted immediately. This is not possible for irrational values of  $\kappa/2$ . Note that this kind of commensurability and incommensurability has also been observed for the periodic chain with this type of interaction [10].

### 3.2. $p, q \in \mathbb{R}$

Without loss of generality, we are going to restrict ourselves to  $p > q$  which implies  $Q < 1$ . We have to distinguish two different situations. If  $\alpha'_- \beta'_+$  equals zero we can adopt the results for the symmetric case with  $F = C = 0$  (see the appendix for details). One has just to exchange  $\alpha_\pm$  and  $\beta_\pm$  by  $\alpha'_\pm$  and  $\beta'_\pm$ . If otherwise  $\alpha'_- \beta'_+ \neq 0$  the situation changes. The energy gaps suggest the partition function for the long chain (2) with boundary terms given by (26), i.e.

$$\mathcal{Z}_{\text{long}} = \text{tr} z^{\frac{2L}{(Q+1/Q)\pi} (H - e_\infty L - f_\infty)} = \frac{2}{\eta(z)} \sum_{m \in \mathbb{Z}/2} z^{2(m+\Delta_x/2)^2 + 2mL\Delta_y} \tag{31}$$

where

$$\Delta_x = \frac{i}{2\pi} \ln \Gamma \quad \Delta_y = \frac{i}{\pi} \frac{Q - Q^{-1}}{Q + Q^{-1}} \tag{32}$$

and

$$\Gamma = (1 - Q^2(1 - 2\alpha_z^2 - 2\alpha'_-\alpha'_+) - 2\alpha_z^2 Q^4) \times (1 - Q^2(1 - 2\beta_z^2 - 2\beta'_-\beta'_+) - 2\beta_z^2 Q^4) / (\alpha_-^2 \beta_+^2 Q^4 (1 + Q^2)^2). \tag{33}$$

Note that the value of  $\Delta_y$  is purely imaginary. Hence the length-dependent term given in the partition function is a phase. Such a term already appeared in the toroidal partition function for the asymmetric model with periodic boundary conditions [13]. Note also that the result (31) simplifies to the partition function we obtained in the Neumann–Neumann case for  $H_{\text{long}}$  if one sets  $Q = 1$  (see (14)).

In [1] we computed the exact ground-state energy on the finite chain for boundaries defined by

$$\alpha_z = \beta_z = 0 \quad \alpha'_+\alpha'_- = \beta'_+\beta'_- = 1. \tag{34}$$

If we introduce the parameter  $\chi'$  via  $\beta'_+ = e^{i\pi\chi'}\alpha'_+$ , then (33) simplifies to

$$\Gamma = (e^{i\pi\chi'} Q^2)^{-2}. \tag{35}$$

Expanding the exact expression obtained in [1] leads to

$$E_0 \sim -\frac{Q + Q^{-1}}{2\pi} L - \frac{Q + Q^{-1} + (Q - Q^{-1})\frac{1}{2} \ln \Gamma}{2\pi} - \frac{(Q + Q^{-1})\pi}{2L} \left( \frac{1}{24} + \frac{(\ln \Gamma)^2}{8\pi} \right). \tag{36}$$

It is only for this case that we can perform the projection onto the (+, +)-sector. We obtain

$$\mathcal{Z} = \frac{1}{\eta(z)} \sum_{m \in \mathbb{Z}} z^{2(m+\chi'/2-i \ln Q/\pi)^2+2mL\Delta_y} \quad \text{for odd } L \tag{37}$$

$$\mathcal{Z} = \frac{1}{\eta(z)} \sum_{m \in \frac{1}{2}(2\mathbb{Z}+1)} z^{2(m+\chi'/2-i \ln Q/\pi)^2+2mL\Delta_y} \quad \text{for even } L. \tag{38}$$

Note that our results for  $H_{\text{long}}$  only apply if (33) is different from zero. If the nominator of  $\Gamma$  vanishes we obtain logarithmic terms in the asymptotic behaviour of the energy gaps similar to those obtained for the symmetric chain. We obtained the fermion energies

$$2\Lambda \sim \frac{Q + Q^{-1}}{2L} \left\{ k\pi \pm \frac{1}{2} [\arg \Delta - i \ln L] \right\} \pm i \frac{Q - Q^{-1}}{2} \tag{39}$$

where

$$\Delta = \frac{2\alpha_-^2 \beta_+^2 Q^4 (1 + Q^2)^2}{2A Q^2 + 4Q^4 (B + E^2) - 6Q^6 (D + 2E^2) + 8E^2 Q^8}. \tag{40}$$

The values of  $A, B, D, E$  are given in (A3). We are not going to consider the case, where the denominator in (40) vanishes.

#### 4. Conclusions

In this paper we considered the spectra of the XX model with boundary fields given by the Hamiltonian  $H$  in (1). In order to obtain our results we also studied the Hamiltonian  $H_{\text{long}}$  defined by (2). Furthermore, we considered the asymmetric XX chain (25). Here we separated two cases. First we considered the case where the values of  $p$  and  $q$  in (25) are given by  $p = e^{i\pi\kappa}/2$  and  $q = e^{-i\pi\kappa}/2$  (this corresponds to Dzyaloshinsky–Moriya interactions). Second we considered the case where  $p$  and  $q$  are real numbers.

For periodic boundary conditions the partition function for  $H$  is given by the partition function of the free boson with periodic boundary conditions (5) [4–6]. The partition function for  $H_{\text{long}}$  with periodic boundary conditions is just the expression (5) multiplied by four. The spectra of the asymmetric chain with Dzyaloshinsky–Moriya interactions have been studied in [10] for free and toroidal boundary conditions, whereas the partition function for real values of  $p$  and  $q$  and periodic boundary conditions was given in [13].

The results we obtained for  $H$  and  $H_{\text{long}}$  can be encoded in terms of the parameters given in (10). For reasons discussed in the text we obtained the energy gaps only for the cases given in table 1. Note that as long as we restrict ourselves to Hermitian boundary terms we studied the most general case. This is not true for non-Hermitian boundaries.

For  $H$  with Hermitian boundaries we obtained the partition functions corresponding to one of the three boson partition functions (7)–(9). However, we also found these partition functions for certain non-Hermitian boundary terms.

We obtained the Neumann–Neumann partition function (8) if all non-diagonal terms are present, where the value of  $\Delta$  in (8) is given by (13). The Dirichlet–Neumann partition function (9) is obtained for boundary terms which satisfy (16). We found the Dirichlet–Dirichlet partition function (7) for two types of boundary terms given by (18), respectively, (17). The value of  $\Delta$  in (7) is given by (19) in both cases. Furthermore, for the case of non-Hermitian boundaries we found a case which is special. For boundary terms given by (20) the partition function is the Dirichlet–Dirichlet partition function (7) multiplied by two, where the value of  $\Delta$  is 0 or  $\frac{1}{2}$  for odd, respectively, even values of the lattice length.

The partition functions for  $H_{\text{long}}$  have also been considered. If all non-diagonal terms are present it is given by (14). For the other cases it is just the partition function of  $H$  multiplied by four. We also computed the values of the free surface energies of  $H_{\text{long}}$  and  $H$  for certain boundary terms. They are given in table 2. In this table we have also given the values of the lowest highest weights which appear in the spectra of  $H_{\text{long}}$  for these boundary terms.

For the last two cases in table 1 we obtained logarithmic corrections to the free surface energy (equation (21)). Here we found also logarithmic terms in the asymptotic behaviour of the energy gaps (equation (22)).

In the case of Dzyaloshinsky–Moriya interactions, we restricted ourselves to Hermitian chains. The value of the phase  $\kappa$  (see (27)) only has an effect on the spectra if non-diagonal boundary terms are present at both ends of the chain. In this case we obtain the Neumann–Neumann partition function (8) if  $\kappa/2$  is a rational number. The value of  $\chi$  in the definition of  $\Delta$  in (13) has just to be exchanged by the expression in (30).

The partition function for the asymmetric chain (25) with real values of  $p$  and  $q$  has only been obtained for one special type of boundaries (see equation (34)). It is given by (37) for  $L$  odd, respectively, by (38) for  $L$  even. The asymptotic behaviour of the ground-state energy for this case is given in (36).

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**Appendix. Determination of the energy gaps**

In [1] we have seen that the spectrum of  $H_{\text{long}}$  is given in terms of free fermions. The fermionic energies  $2\Lambda_n$  are given by

$$2\Lambda_n = \frac{1}{2}(x_n + x_n^{-1}) \tag{A1}$$

where the  $x_n$  are the roots of the polynomial

$$\begin{aligned} p(x^2) = & [x^{4L+8} + 1 - A(x^{4L+6} + x^2) + (B + E^2)(x^{4L+4} + x^4) \\ & + (D + 2E^2)(x^{4L+2} + x^6) + E^2(x^{4L} + x^8) - 2E(x^{2L+8} + x^{2L}) \\ & + ((A - B - D - 1)/2 - (-1)^L C - 2E^2)(x^{2L+6} + x^{2L+2}) \\ & + (A - B - D - 1 + 2(-1)^L C + 4E - 4E^2)x^{2L+4}] / (x^2 - 1)^2 \end{aligned} \tag{A2}$$

where the coefficients appearing in (A2) are functions of the boundary parameters

$$\begin{aligned} A = 2(\alpha_- \alpha_+ + \beta_- \beta_+ + \alpha_z^2 + \beta_z^2 - 1) \quad C = \alpha_-^2 \beta_+^2 + \alpha_+^2 \beta_-^2 \\ B = (2\alpha_- \alpha_+ - 1)(2\beta_- \beta_+ - 1) + 4\beta_z^2(\alpha_- \alpha_+ - 1) + 4\alpha_z^2(\beta_+ \beta_- - 1) \\ D = \beta_z^2(4\alpha_- \alpha_+ - 2) + \alpha_z^2(4\beta_+ \beta_- - 2) \quad E = 2\alpha_z \beta_z. \end{aligned} \tag{A3}$$

Since there appear four zeros for each fermion, namely  $x_n, x_n^{-1}, -x_n$  and  $-x_n^{-1}$ , the polynomial yields  $L + 1$  fermionic energies (see [1] for details). In addition to these fermions there always exists a fermion with energy  $2\Lambda_0 = 0$ , which we called a ‘spurious’ zero mode. All possible combinations of these  $L + 2$  fermions build up the spectrum of  $H_{\text{long}}$ . The spectrum of  $H$  is then obtained by excluding the ‘spurious’ zero mode from the set of fermion energies and then taking the sector with an even or with an odd number of fermions being excited with respect to the vacuum. How to decide whether one has to pick up the even or the odd sector has been discussed in detail in [1].

Since in this paper we are interested into the large- $L$  behaviour of the low-lying energy levels, we look for the asymptotics of the zeros of  $p(x^2)$  in the vicinity of the point  $x = \pm i$  using the ansatz  $x = e^{i\pi/2 - i\phi/L}$ , where we assume  $\phi$  to be a constant in leading order. For the first four cases given in table 1 we obtained the following equations:

- $F \neq 0$

$$\cos(2\phi) + \frac{2C}{F} = 0 \tag{A4}$$

- $F = C = 0, G \neq 0$

$$\phi \sin(2\phi) = 0 \tag{A5}$$

- $F = C = G = 0, K \neq 0$

$$\phi^2 \left[ \cos(2\phi) + (-1)^{L+1} \frac{J}{K} \right] = 0 \tag{A6}$$

- $F = C = G = K = J = 0$

$$\phi^4 \exp(2i\phi) = (-1)^L. \tag{A7}$$

Solving these equations for  $\phi$  yields the energy gaps (cf (A1)) in leading order. We obtained the following expressions:

- $F \neq 0$

$$2\Lambda \sim \frac{1}{L} \left[ \frac{1}{2}(2n - 1)\pi \pm \frac{1}{2} \arccos \left( \frac{2C}{F} \right) \right] \quad 1 \leq n \tag{A8}$$

- $F = C = 0, G \neq 0$

$$2\Lambda \sim \frac{1}{L} \frac{n}{2} \pi \quad 0 \leq n \tag{A9}$$

- $F = C = G = 0, K \neq 0$

$$2\Lambda \sim \frac{1}{L} \left[ \frac{2n - 1}{2} \pi \pm \frac{1}{2} \arccos \left( (-1)^{L+1} \frac{J}{K} \right) \right] \quad 1 \leq n. \tag{A10}$$

In addition to these modes there appears an additional zero mode.

- $F = C = G = K = J = 0$

$$2\Lambda \sim \frac{1}{L} n \pi \quad 1 \leq n \quad \text{for } L \text{ even} \tag{A11}$$

$$2\Lambda \sim \frac{1}{L} \frac{2n - 1}{2} \pi \quad 1 \leq n \quad \text{for } L \text{ odd.} \tag{A12}$$

Furthermore, we found three additional zero modes for  $L$  even and two additional zero modes for  $L$  odd.

For the last two cases in table 1 the asymptotic zeros of the polynomial can only be found using the ansatz  $x = e^{i\pi/2 - i\phi/L}$  if we assume the imaginary part of  $\phi$  to diverge as  $L$  goes to infinity. Hence we generalize our ansatz to  $x = e^{i\pi/2 - i\phi(L)/L}$ , where  $\phi(L)$  is a complex function. Furthermore, we assume  $\lim_{L \rightarrow \infty} \phi(L)/L = 0$  and  $\lim_{L \rightarrow \infty} e^{-i\phi(L)} = 0$ . The second assumption will be explained shortly. In both cases our ansatz leads to the solution of an equation of the form

$$ae^{-2i\phi(L)} \left[ 1 + O\left(\frac{\phi(L)}{L}\right) \right] + \frac{2i\phi(L)}{L} \left[ b + O\left(\frac{\phi(L)}{L}\right) \right] = 0. \tag{A13}$$

From this expression one can see that our second assumption is indeed necessary to solve this equation, since otherwise the first term would be finite for all values of  $L$ , whereas the second term vanishes as  $L$  goes to infinity. Neglecting the terms of order  $\phi(L)/L$  this equation is solved in terms of the so-called Lambert W function  $\mathcal{L}$  which is defined by the property  $\mathcal{L}(x) e^{\mathcal{L}(x)} = x$ . We obtain

$$\phi(L) = -i\mathcal{L}(\Delta L)/2 \quad \text{where } \Delta = -\frac{a}{b}. \tag{A14}$$

The asymptotic behaviour of  $\mathcal{L}$  is well known [17], i.e.

$$\mathcal{L}(L) \sim 2ik\pi + \ln L - \ln(\ln L + 2i\pi k) + \dots \tag{A15}$$

Note that this expression is in accordance with the assumptions we made concerning the asymptotic behaviour of  $\phi(L)$ .

In this paper we also considered the asymmetric chain, which is similar to the symmetric chain with length-dependent boundary parameters (cf equation (26)). This length dependence enters the polynomial (A2) only via the coefficient  $C$ , which becomes

$$C = \alpha_-^2 \beta_+^2 Q^{2-2L} + \alpha_+^2 \beta_-^2 Q^{2L-2}. \tag{A16}$$

For  $Q < 1$  (the case considered in section 3.2) the first term on the right-hand side of (A16) diverges exponentially, whereas the second term vanishes exponentially as a function of the

lattice length  $L$ . Hence we have to distinguish two different situations. If  $\alpha'_- \beta'_+$  equals zero we may find the asymptotic zeros of the polynomial as for the symmetric case with  $F = C = 0$ . If otherwise  $\alpha'_- \beta'_+ \neq 0$  then  $C$  diverges as  $L$  is increased. This has to be compensated by modifying our ansatz to  $x = e^{i\pi/2 - i\phi/L + \ln Q}$ . This works as long as the nominator of  $\Gamma$  in (33) is different from zero. Otherwise we have to modify our ansatz another time to  $x = e^{i\pi/2 - i\phi(L)/L + \ln Q}$ , where  $\lim_{L \rightarrow \infty} \phi(L)/L = 0$  and  $\lim_{L \rightarrow \infty} e^{-i\phi(L)} = 0$ . This leads again to an equation of the form (A13) which can be solved as described above.

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