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New results for the XX model with boundaries

Birgit Wehefritz-Kaufmann

Physics Department, University of Connecticut, U-3046, 2152 Hillside Road, Storrs, CT 06269-3046, USA

E-mail: kaufmann@phys.uconn.edu

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Abstract
In this paper, we study the XX model with particular non-diagonal boundaries. Using a fermionization technique for an extended version of this chain we are able to present a new operator which commutes with the extended and also the original Hamiltonian. It is a highly non-trivial conserved quantity in the spin-chain formalism which gives rise to an interesting combinatorial partition function.

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Introduction

The object of study of this paper is a special case of the Hamiltonian describing the XX model with diagonal and non-diagonal boundaries that was extensively studied in [1–4]:

$$H_{\text{boundary}} = \frac{1}{2}\sum_{j=1}^{L-1}\left[\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+\right] + \frac{1}{\sqrt{8}}\left[\alpha_-\sigma_1^- + \alpha_+\sigma_1^+ + \alpha_z\sigma_1^z + \beta_+\sigma_L^+ + \beta_-\sigma_L^- + \beta_z\sigma_L^z\right]. \tag{1}$$

Recently, there has been a lot of interest in models with boundary terms due to the fact that they can be linked to quite diverse areas of physics. For instance, if σ_z terms are added into the bulk, i.e. one looks at the XXZ model, the Hamiltonian with boundary terms as above can be connected to a raise and peel model that describes a growing and fluctuating interface [5]. In that model, the boundary parameters represent basic physical quantities. This slightly more general model also has connections to many different topics in mathematical physics, such as representation theory of the Temperley–Lieb algebra [6], loop models [7] and combinatorics [8]. There are also interesting results which surprisingly relate spectra of spin chains with different boundary terms to each other [9]. Moreover, there are many more interesting physical phenomena for boundary XXZ chains [10–15], to name a few. Depending on the choice of boundary conditions there are several tools one can use to find analytic solutions such as duality transformations and 'hidden' translational invariance [16–18], which allow one to extend the use of Jordan–Wigner transformations to the boundary case, field theory [19] or quantum group approaches [7, 20, 21]. Each of these approaches is finely tuned to the particular choice of boundary terms. In our case, we use the technique established in [1] which consists of solving a *larger* chain using fermionization and then 'projecting' onto the original smaller chain, which itself *is not* solvable simply by fermionization. Although this technique is different from those mentioned above and applies in a different situation, we comment on intriguing similarities and open questions on the interrelation of the different approaches and situations in the conclusion.

In the following, we will focus on the particular choice of boundary conditions given by the parameters $\alpha^+ = \alpha^- = 1, \alpha^z = \beta^z = 0, \beta^\pm = \mathrm{e}^{\pm\mathrm{i}\chi}$ (where χ is a real parameter with $0 \leqslant \chi \leqslant \frac{\pi}{2}$) in (1), which results in the following expression for the Hamiltonian:

$$H = \frac{1}{2}\sum_{j=1}^{L-1}\left[\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+\right] + \frac{1}{\sqrt{8}}\left[\sigma_1^- + \sigma_1^+ + \exp(\mathrm{i}\chi)\sigma_L^+ + \exp(-\mathrm{i}\chi)\sigma_L^-\right]. \tag{2}$$

Our goal in this paper is to study the hidden symmetries of the spin chain given by equation (2) with non-diagonal boundaries. In particular, we are going to show how to construct a highly non-trivial operator that commutes with the Hamiltonian above. The basic idea is to use the fermionization techniques of [1] to explicitly calculate the transformation from a spin chain to the free fermion case and then use the inverse transform on the fermionic number operator. This is a formidable calculation, since it not only involves the general setup for the diagonalization, but also the full calculation of the basis which diagonalizes the Clifford operators [1, 22]. In order to be explicit about this, we will first briefly summarize the results of [1], on how an extension of the Hamiltonian given by equation (1) can be written as a fermionic model and how one can extract the information about the original Hamiltonian via a 'projection'. Armed with these tools, we can explicitly construct an operator that naturally commutes with the Hamiltonian.

The paper is organized as follows. In paragraph 1, we review the diagonalization techniques of [1]. In paragraph 2, we specialize this general setup to the special values given by our particular choice of boundaries. For this choice of parameters, the characteristic polynomial factorizes and that allows us to explicitly calculate all the necessary data. In section 3, we use the knowledge of the transformation operators in order to transform the fermionic number operator into the spin-chain representation. Finally, we study the thermodynamic limit of the partition function on the super-selection sectors which are defined by this conserved quantity.

1. Diagonalization via extension

We will now review how to treat the spin chain (2) according to the program outlined in [1]. The process consists of five steps. The first is to elongate the chain to obtain a spin chain which is diagonalizable. The next three steps are transformations which bring the chain into the form of free fermions and the last step is the identification of the original spin chain as a sub-sector of the larger theory and the subsequent projection of this sub-sector onto the smaller original chain. In order to do the calculation of the next paragraph we will need to explicitly keep track of all these transformations.

1.1. Step one and five: extending the chain and 'projecting' to the original chain

From now on we regard the Hamiltonian of equation (2), that is we fix $\alpha^+ = \alpha^- = 1, \alpha^z = \beta^z = 0, \beta^\pm = e^{\pm i\chi}$.

A Hamiltonian can be diagonalized in terms of free fermions if it can be written as a bilinear expression in $\sigma^\pm$-matrices, with nearest neighbour interaction, by applying the standard fermionization techniques [22–24]. Since the Hamiltonian of interest given by equation (2) is not of this form, we add one lattice site at each end of the chain, site 0 and site $L+1$ as in [25] to obtain an expression which is indeed bilinear in $\sigma^\pm$-matrices for H. After extending the Hamiltonian by these two sites and making it quadratic, it reads

$$H_{\text{long}} = \frac{1}{2}\sum_{j=1}^{L-1}\left[\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+\right] + \frac{1}{\sqrt{8}}\left[\sigma_0^x\sigma_1^- + \sigma_0^x\sigma_1^+ + \exp(i\chi)\sigma_L^+\sigma_{L+1}^x + \exp(-i\chi)\sigma_L^-\sigma_{L+1}^x\right]. \tag{3}$$

As σ_0^x and σ_{L+1}^x commute with H_{long}, the spectrum of H_{long} decomposes into four sectors $(++, +-, -+, --)$ corresponding to the eigenvalues ± 1 of σ_0^x and σ_{L+1}^x. Now the original Hamiltonian H is the restriction of H_{long} onto the $(+,+)$ eigenspace of $\left(\sigma_0^x, \sigma_{L+1}^x\right)$. The eigenvectors of the original model H can be retrieved by first restricting to the $(++)$ sector and then projecting onto the original chain. See [1] for more details about this. We will not need the eigenvectors of the Hamiltonian in our calculations, but we will need the explicit transformation of the Hamiltonian into free fermions in order to back transform our conserved quantity into the spin picture.

We will now explain the different transformation steps needed in order to diagonalize H of equation (2).

1.2. Step two: Jordan–Wigner transformation

For the first transformation, we will use the Majorana representation of the lattice $s = 1/2$ spin operators as in [23, 26] (see also [16, 17] for other chains with boundary terms diagonalized by using a Jordan–Wigner transformation), set

$$\tau_j^{+,-} = \left(\prod_{i=0}^{j-1}\sigma_i^z\right)\sigma_j^{x,y}. \tag{4}$$

As is well known, these operators obey the anticommutation relations of a Clifford algebra $\left\{\tau_m^\mu, \tau_n^\nu\right\} = 2\delta_{nm}^{\mu\nu}$. Rewriting H_{long} in terms of $\tau_j^{+,-}$, we obtain the following bilinear expression:

$$H_{\text{long}} = -\sum_{\mu,\nu=\pm 1}\sum_{j=1}^{L-1} F^{\mu,\nu}\tau_j^\mu\tau_{j+1}^\nu + G^{\mu,\nu}\tau_0^\mu\tau_1^\nu + K^{\mu,\nu}\tau_L^\mu\tau_{L+1}^\nu, \tag{5}$$

where F, G and K are 2×2 matrices which have the general form $A = \begin{pmatrix} A^{--} & A^{-+} \\ A^{+-} & A^{++}\end{pmatrix}$ meaning that the jth term reads $\sum_{(\mu,\nu)} A^{(\mu,\nu)}\tau_j^\mu\tau_{j+1}^\nu$. Their particular values are

$$F = \frac{1}{4}\begin{pmatrix} 0 & i \\ -i & 0\end{pmatrix}, \qquad G = \frac{1}{2}\begin{pmatrix} 0 & \frac{2i}{\sqrt{8}} \\ 0 & 0\end{pmatrix}, \qquad K = \frac{1}{2}\begin{pmatrix} 0 & \frac{i}{\sqrt{8}}2\cos(\chi) \\ 0 & \frac{i}{\sqrt{8}}2\sin(\chi)\end{pmatrix} \tag{6}$$

1.3. Step three: diagonalizing the Clifford operators

Now that we have presented H_{long} as a quadratic form in Clifford operators, we go on to diagonalize this form. Note that this quadratic form can be regarded an even form on the odd Clifford operators $\tau_j^{\pm}$ or equivalently as an odd form on the vector space underlying the Clifford algebra which can be thought of as being spanned by the $\tau_j^{\pm}$, see e.g. [22]. Adopting the latter point of view, we apply a linear transformation to the $\tau_j^{+,-}$ operators to diagonalize the Hamiltonian, but we have the additional restriction that the commutation relations of the images of the transformed operators in the Clifford algebra are another set T_n^+, T_n^- of Clifford operators, that is they still satisfy the Clifford relations

$$\left\{T_m^{\mu}, T_n^{\nu}\right\} = 2\delta_{nm}^{\mu\nu}. \tag{7}$$

To this end, we write out the explicit form of this linear transformation

$$T_n^{\gamma} = \sum_{j=0}^{L+1} \sum_{\mu=\pm 1} \left(\psi_n^{\gamma}\right)_j^{\mu} \tau_j^{\mu} \tag{8}$$

where $\gamma = \pm 1$ and $\left(\left(\psi_n^{\gamma}\right)_j^{\mu}\right)_{(\gamma n),(\mu j)}$ is the transformation matrix in the vector space spanned by the τ_j^{μ}. The condition on this transformation is two-fold: first the operators T are new Clifford operators and second H_{long} takes the simple 'diagonal' form

$$H_{\text{long}} = \sum_{n=0}^{L+1} \Lambda_n \mathrm{i} T_n^- T_n^+. \tag{9}$$

The first condition implies that the operator $\mathrm{i}T_n^- T_n^+$ has eigenvalues ± 1 and thus the spectrum of H_{long} is given by all possible $\mathbb{Z}/2\mathbb{Z}$ combinations that is sums over the Λ_n with coefficients +1 or -1 and hence is known as soon as the Λ_n are.

Using the second condition or equivalently computing the commutator $\left[H_{\text{long}}, T_n^{\pm}\right]$ using the two different presentations of H_{long} given by equations (9) and (5) and then equating both results, one finds that the eigenvalues Λ_n and the vectors

$$\psi_n^{\gamma} = \left(\left(\psi_n^{\gamma}\right)_0^-, \left(\psi_n^{\gamma}\right)_0^+, \ldots, \left(\psi_n^{\gamma}\right)_{L+1}^-, \left(\psi_n^{\gamma}\right)_{L+1}^+\right), \qquad \gamma = \pm \tag{10}$$

are given by the solutions of the following equations:

$$M\psi_n^+ = -\mathrm{i}\Lambda_n \psi_n^-, \qquad M\psi_n^- = \mathrm{i}\Lambda_n \psi_n^+, \tag{11}$$

where M is the $(2L+4) \times (2L+4)$ matrix given by

$$M = \begin{pmatrix} 0 & G & & & & \\ -G^T & 0 & F & & & \\ & -F^T & 0 & F & & \\ & & \cdots & \cdots & \cdots & \\ & & & -F^T & 0 & K \\ & & & & -K^T & 0 \end{pmatrix}. \tag{12}$$

Taking the linear combinations

$$\phi_n^+ = \psi_n^+ - \mathrm{i}\psi_n^-, \qquad \phi_n^- = \psi_n^+ + \mathrm{i}\psi_n^- \tag{13}$$

allows one to rewrite these equations as the eigenvalue problem

$$M\phi_n^{\pm} = \pm\Lambda_n \phi_n^{\pm}. \tag{14}$$

Observe that M has $2L+4$ eigenvalues as expected, since it is a transformation in the space spanned by the τ_j^{μ}, whereas H_{long} has only length $L+2$ and one thus needs 2^{L+2} eigenvalues. In the fermionic language one needs $L+2$ Fermions, which matches up nicely, since considering equation (14) one can see that with the appearance of each eigenvalue Λ_n one also gets the negative eigenvalue $-\Lambda_n$. This is not a coincidence, but follows from the ambiguity in the basis for the diagonalization of a quadratic form [22]. As mentioned above, the spectrum of H_{long} is given by all linear combinations of Λ_n with coefficients ± 1 (see equation (9)) and thus can be retrieved from the eigenvalues of M by choosing from each pair of eigenvalues $\pm\Lambda_n$ one value as basis element for the $\mathbb{Z}/2\mathbb{Z}$ linear combinations. The choice we will make for the physically positive excitations will be those Λ with a positive real part.

1.4. Step four: transforming to free fermions

Finally, to express the spectrum of H_{long} in terms of free fermions, we will yet again make a third transformation and write the expression for the Hamiltonian in terms of fermionic operators b_n and a_n which satisfy

$$\{b_n, a_m\} = \delta_{n,m}, \qquad \{b_n, b_m\} = 0, \qquad \{a_n, a_m\} = 0. \tag{15}$$

These are obtained from the Clifford operators T_n^+ and T_n^- in the following standard fashion:

$$b_n = \tfrac{1}{2}\left(T_n^+ + \mathrm{i}T_n^-\right); \qquad a_n = \tfrac{1}{2}\left(T_n^+ - \mathrm{i}T_n^-\right). \tag{16}$$

Plugging in these expressions, H_{long} reads

$$H_{\text{long}} = \sum_{n=0}^{L+1} 2\Lambda_n b_n a_n - \sum_{n=0}^{L+1} \Lambda_n = \sum_{n=0}^{L+1} 2\Lambda_n N_n + E_0, \tag{17}$$

where E_0 is the ground state energy of the system and $N_n := b_n a_n$ is the number operator (with eigenvalues 0 and 1) for the fermion with energy $2\Lambda_n$.

The fermionic operators a_m, b_m can be expressed in terms of the τ_j^+, τ_j^--operators by using the eigenvectors of M and equation (8)

$$a_m = \frac{1}{2}\left(T_m^+ - \mathrm{i}T_m^-\right) = \frac{1}{2}\sum_{j=0}^{L+1}\sum_{\mu=\pm 1} \left(\phi_m^+\right)_j^\mu \tau_j^\mu \tag{18}$$

$$b_m = \frac{1}{2}\left(T_m^+ + \mathrm{i}T_m^-\right) = \frac{1}{2}\sum_{j=0}^{L+1}\sum_{\mu=\pm 1} \left(\phi_m^-\right)_j^\mu \tau_j^\mu. \tag{19}$$

2. Explicit calculation of the spectrum and the transformation

Using the procedure described in [1], the eigenvectors ϕ yielding the similarity transformation can also be explicitly calculated as follows: we will index the vectors $(\phi_k^\pm)$ analogously to equation (10), that is we take (13) componentwise. The eigenvalue problem given by equation (14) is then equivalent to a set of recurrence relations. In the bulk the equations read

$$\left.\begin{aligned} \tfrac{\mathrm{i}}{4}\left(\left(\phi_k^\pm\right)_j^+ + \left(\phi_k^\pm\right)_{j+2}^+\right) &= \pm\Lambda_k\left(\phi_k^\pm\right)_{j+1}^- \\ -\tfrac{\mathrm{i}}{4}\left(\left(\phi_k^\pm\right)_j^- + \left(\phi_k^\pm\right)_{j+2}^-\right) &= \pm\Lambda_k\left(\phi_k^\pm\right)_{j+1}^+ \end{aligned}\right. \qquad (1 \leqslant j \leqslant L-2). \tag{20}$$

Using the auxiliary expressions

$$\varphi_j^\pm = \left(\phi_k^\pm\right)_j^- + \mathrm{i}\left(\phi_k^\pm\right)_j^+, \qquad \overline{\varphi}_j^\pm = \left(\phi_k^\pm\right)_j^- - \mathrm{i}\left(\phi_k^\pm\right)_j^+ \tag{21}$$

equations (20) take the simple form:

$$\tfrac{1}{4}(\varphi_j + \varphi_{j+2}) = \lambda\varphi_{j+1}, \qquad -\tfrac{1}{4}(\overline{\varphi}_j + \overline{\varphi}_{j+2}) = \lambda\overline{\varphi}_{j+1}. \tag{22}$$

Here we used the short-hand notation λ to simultaneously treat the two cases $\lambda = \pm\Lambda_k$. The functions φ_j and $\overline{\varphi}_j$ are accordingly short hand and refer to φ_j^+ and $\overline{\varphi}_j^+$ for $\lambda = \Lambda_k$ and to φ_j^- and $\overline{\varphi}_j^-$ for $\lambda = -\Lambda_k$. From now on we will keep k fixed and omit all subscripts referring to k. Using the auxiliary variable x which is related to λ via

$$\lambda = \tfrac{1}{4}(x + x^{-1}), \tag{23}$$

the general solution of the bulk equations (22) for fixed k and $\lambda \neq \pm\frac{1}{2}$ is given by

$$\varphi_j = ax^j + bx^{-j}, \qquad \overline{\varphi}_j = g(-x)^j + f(-x)^{-j}, \tag{24}$$

where $1 \leqslant j \leqslant L$. The four parameters a, b, g, f and the yet undetermined components $\varphi_0, \overline{\varphi}_0, \varphi_{L+1}, \overline{\varphi}_{L+1}$ together with the eigenvalues λ are all fixed by the boundary equations (26)–(29), up to the normalization constants of the eigenvectors. For $\lambda = \pm\frac{1}{2}$ the general solution is

$$\varphi_j = a(\pm 1)^j + b(\pm 1)^j j, \qquad \overline{\varphi}_j = g(\mp 1)^j + f(\mp 1)^j j. \tag{25}$$

Note that looking at the matrix M there are two obvious eigenvectors $(0, 1, 0, \ldots)$ and $(\ldots, 0, 1, 0)$. We will set $\varphi_0 = \overline{\varphi}_0$ and $\overline{\varphi}_{L+1} = -\overline{\varphi}_{L+1}$ and exclude these cases from the further discussions of the boundary equations. Thus we are looking for additional $2L + 2$ linearly independent solutions.

From the left boundary, we obtain the equations

$$\varphi_0 = \overline{\varphi}_0, \qquad \lambda\varphi_0 = \tfrac{1}{\sqrt{32}}(\varphi_1 - \overline{\varphi}_1) \tag{26}$$

and

$$\lambda\varphi_1 = \tfrac{1}{\sqrt{8}}\varphi_0 + \tfrac{1}{4}\varphi_2, \qquad \lambda\overline{\varphi}_1 = -\tfrac{1}{\sqrt{8}}\overline{\varphi}_0 - \tfrac{1}{4}\overline{\varphi}_2. \tag{27}$$

And from the right boundary, we obtain analogously

$$\lambda\varphi_L = \tfrac{1}{\sqrt{8}}\,\mathrm{e}^{\mathrm{i}\chi}\varphi_{L+1} + \tfrac{1}{4}\varphi_{L-1}, \qquad \lambda\overline{\varphi}_L = -\tfrac{1}{\sqrt{8}}\,\mathrm{e}^{-\mathrm{i}\chi}\overline{\varphi}_{L+1} - \tfrac{1}{4}\overline{\varphi}_{L-1} \tag{28}$$

and

$$\lambda\varphi_{L+1} = \tfrac{1}{\sqrt{32}}(\mathrm{e}^{\mathrm{i}\chi}\overline{\varphi}_L + \mathrm{e}^{-\mathrm{i}\chi}\varphi_L), \qquad \varphi_{L+1} = -\overline{\varphi}_{L+1}. \tag{29}$$

Expressing the equations in the new variable x and assuring that the linear equations (26)–(29) have a solution, we obtain the characteristic polynomial of these equations and hence of M:

$$p(x) = (1 - sx^{2L+2})(1 - 1/sx^{2L+2}) \tag{30}$$

with $s = \exp(2\mathrm{i}\chi)$. We can explicitly solve for the roots x_n, i.e. $p(x_n) = 0$, to obtain

$$x_n = \exp\left(-\frac{\mathrm{i}\pi}{2} + \frac{\mathrm{i}\chi}{L+1} + \frac{(2n+1)\mathrm{i}\pi}{2L+2}\right), \qquad n = 0, \ldots, L \tag{31}$$

and therefore

$$\Lambda_n = \frac{1}{2}\sin\left(\frac{\chi}{L+1} + \frac{(2n+1)}{L+1}\frac{\pi}{2}\right), \qquad n = 0, \ldots, L. \tag{32}$$

Using these equations we can write out the dependence of the components of the ϕ-vectors in terms of the roots x_n: for $j = 1, \ldots, L$

$$
\begin{aligned}
(\phi_n^-)_0^- &= \frac{x_n}{\sqrt{2L+2}}, & (\phi_n^+)_0^- &= -\frac{x_n}{\sqrt{2L+2}}\\
(\phi_n^-)_0^+ &= 0, & (\phi_n^+)_0^+ &= 0\\
(\phi_n^-)_j^- &= \frac{1}{2\sqrt{L+1}}\big((-1)^j x_n^{j+1} + x_n^{-j+1}\big), & (\phi_n^+)_j^- &= \frac{1}{2\sqrt{L+1}}\big(-x_n^{j+1} + x_n^{-j+1}(-1)^{j+1}\big);\\
(\phi_n^-)_j^+ &= \frac{-\mathrm{i}}{2\sqrt{L+1}}\big((-1)^j x_n^{j+1} - x_n^{-j+1}\big), & (\phi_n^+)_j^+ &= \frac{-\mathrm{i}}{2\sqrt{L+1}}\big(-x_n^{j+1} - x_n^{-j+1}(-1)^{j+1}\big);\\
(\phi_n^-)_{L+1}^- &= 0, & (\phi_n^+)_{L+1}^- &= 0\\
(\phi_n^-)_{L+1}^+ &= \frac{\mathrm{i}x_n^{L+2}}{\sqrt{2L+2}\exp(\mathrm{i}\chi)}, & (\phi_n^+)_{L+1}^+ &= \frac{\mathrm{i}x_n^{L+2}}{\sqrt{2L+2}\exp(\mathrm{i}\chi)}.
\end{aligned}
$$

The thought after transformation ϕ is then given by plugging in the different values of x_n.

3. The conserved quantity

The following operator counts the number of fermions present for H_{long}:

$$F_{\text{long}} = \sum_{n=1}^{L+1} N_n = \sum_{n=0}^{L} b_n a_n = \frac{1}{4}\sum_{n=0}^{L}\sum_{j=0}^{L+1}\sum_{k=0}^{L+1}\sum_{\mu=\pm1}\sum_{\nu=\pm1} (\phi_n^-)_j^{\mu}(\phi_n^+)_k^{\nu}\tau_j^{\mu}\tau_k^{\nu}. \tag{33}$$

Here N_n are as above the fermionic number operators (with eigenvalues 0 and 1) corresponding to the fermionic excitations with energies given by equation (32). This is an operator that naturally commutes with H_{long} and has integer eigenvalues. It turns out that this operator can even be written down for H, leading to a highly non-trivial conservation law when expressed in the basis of sigma matrices. This latter 'projection' is possible since F_{long} takes on the form

$$F_{\text{long}} = \sigma_0^x \otimes F_1 \otimes \sigma_{L+1}^x + \sigma_0^x \otimes F_2 \otimes \mathrm{id} + \mathrm{id} \otimes F_3 \otimes \sigma_{L+1}^x + \mathrm{id} \otimes F_4 \otimes \mathrm{id} \tag{34}$$

and hence by restricting and then projecting we obtain the operator $F = \sum_{i=1}^{4} F_i$ which commutes with H.

Note that the operator N_0 is missing from the above equation. This is due to the fact that the long chain has an additional symmetry which results in a zero mode that is not present in the short chain, which does not possess this symmetry. The corresponding zero mode excitation is not part of the original chain and it does not contribute to its spectrum [1]. Or in other words it is not an excitation of the original chain. Hence we omit it in the fermion count for the short chain. If this operator were present, the projection would also not be possible.

Plugging in the eigenvectors $\phi_n^{\pm}$ that yield the transformation matrix given in equation (32), summing over n and using equation (4), we can express operator F_{long} in the basis of σ-matrices. After 'projecting' this operator onto the original chain as explained above, one obtains the following expression:

$$
\begin{aligned}
F = \frac{1}{4L+4} \sum_{\substack{j,k=1\\ j+k\ \text{odd},\, j<k}}^{L} (-1)^{\frac{j+k+1}{2}} \left(\sigma_{j+1}^z \ldots \sigma_{k-1}^z\right) \Bigg[\left(\frac{\sin\left(\frac{\chi(j-k)}{L+1}\right)}{\sin\left(\frac{\pi(j-k)}{2L+2}\right)} + \frac{\sin\left(\frac{\chi(j+k)}{L+1}\right)}{\sin\left(\frac{\pi(j+k)}{2L+2}\right)} \right) \\
\times \left(\sigma_j^x\sigma_k^y - \sigma_j^y\sigma_k^x\right) + \left(\frac{\cos\left(\frac{\chi(j+k)}{L+1}\right)}{\sin\left(\frac{\pi(j+k)}{2L+2}\right)} \right) \left(\sigma_j^y\sigma_k^y - \sigma_j^x\sigma_k^x\right) \Bigg] + \frac{1}{\sqrt{8}(L+1)}
\end{aligned}
$$

$$\times \left\{ \sum_{\substack{k=1 \\ k \text{ odd}}}^{L-1} (-1)^{\frac{k+1}{2}} \left[\frac{\cos\left(\frac{\chi k}{L+1}\right)}{\sin\left(\frac{\pi k}{2L+2}\right)} \sigma_1^z \sigma_2^z \ldots \sigma_{k-1}^z \sigma_k^x \right] \right.$$
$$\left. + \sum_{\substack{k=2 \\ k \text{ even}}}^{L} \left[(-1)^{\frac{L+k+2}{2}} \frac{\cos\left(\frac{\chi k}{L+1}\right)}{\cos\left(\frac{\pi k}{2L+2}\right)} \sigma_k^x + (-1)^{\frac{k+L}{2}} \frac{\sin\left(\frac{\chi k}{L+1}\right)}{\cos\left(\frac{\pi k}{2L+2}\right)} \sigma_k^y \right] \left(\sigma_{k+1}^z \ldots \sigma_{L-1}^z \sigma_L^z\right) \right\}. \tag{35}$$

It is clear that it would be next to impossible to find this operator relying solely on the spin-chain picture. Since it appears to be highly non-standard it looks to be all the more a very interesting expression.

To understand the physical nature of the number of fermions in the thermodynamic limit, we define the partition function of H_{long} in the sector with m fermions in the limit where L goes to ∞ as

$$Z_m = \lim_{L\to\infty} \left\{ \operatorname{tr} z^{\frac{L}{\pi} \sum_{n=0}^{L} 2\Lambda_n N_n} \right\} \tag{36}$$

with the constraint $\sum_{n=0}^{L} N_n = m$ where m is some fixed positive integer (counting the number of fermions). Here N_n denote the eigenvalues (0 or 1) of the fermionic number operators.

Since $\lim_{L\to\infty}\left(\frac{2L\Lambda_n}{\pi}\right) = \frac{\chi}{\pi} + \frac{1}{2} + n$ this leads to

$$Z_m = z^{\frac{m\chi}{\pi} + \frac{m}{2}} \sum_{n_1, n_2, \ldots, n_m} z^{n_1 + n_2 + \cdots + n_m}$$
$$= z^{\frac{m\chi}{\pi} + \frac{m}{2}} \left(\sum_l p_m(l) z^l + \sum_l p_{m-1}(l) z^l \right). \tag{37}$$

Here $p_m(l)$ counts the number of ways the integer l can be expressed as a sum of m distinct integers. The second term involving p_{m-1} takes into account that one of the n_i in the sum before might be zero. Since

$$\sum_l p_m(l) z^l = \frac{z^{\frac{m(m+1)}{2}}}{(1-z)(1-z^2)\cdots(1-z^m)}, \tag{38}$$

we obtain

$$Z_m = z^{\frac{m\chi}{\pi} + \frac{m}{2}} \left(\frac{z^{\frac{m(m+1)}{2}} + (1-z^m) z^{\frac{(m-1)m}{2}}}{(1-z)(1-z^2)\cdots(1-z^m)} \right)$$
$$= z^{\frac{m\chi}{\pi} + \frac{m}{2}} \left(z^{\frac{m(m+1)}{2}} + (1-z^m) z^{\frac{(m-1)m}{2}} \right) \frac{\prod_{l=1}^{\infty}(1 - z^m z^l)}{\eta(z)}. \tag{39}$$

Although the coefficients are explicit in terms of partitions of a given number satisfying certain conditions, it seems that not much else is known about this generating series [27]. In particular it would be desirable to find new expressions for the nominator in (39) and study the modular properties of the partition function.

4. Conclusion

Using the correspondence between spin-chains Hamiltonians and fermionic systems and its extension to the case of non-trivial boundary terms, we have found a new operator that commutes with our original Hamiltonian. The is a two-fold surprise. First it is not *a priori* clear that the total fermion operator descends to the original chain. Second, the expression in terms of the σ-matrices, that is the conserved quantity in the spin system is highly non-trivial.

It is interesting to note that there are also quite involved symmetries for the XXZ chain which come from field theory considerations [19] or from quantum group considerations [7, 20, 21]. To our knowledge there is no obvious relation between the conserved charge found in those studies for the XXZ chain and the one we derived for the XX model, especially since the boundary conditions are very different. However, their relation is an interesting open question especially in view of the fact that our theory behaves as a free boson with Neumann–Neumann boundary conditions in the thermodynamic limit [2] and these are also the boundary conditions used in [19]. Furthermore the ground state energies derived in [17, 18] are reminiscent of the coefficients of equation (35), so that one might speculate that there is some hidden translational symmetry. This would be by no means obvious since our system is not periodic and has different boundary conditions on both ends. One clue to the existence of a 'hidden' symmetry like this is the fact that our spectrum is given by the even fermion excitations of $L+1$ fermions. In terms of Clifford operators there is an embedding of the Clifford algebra on a $(2L+1)$-dimensional vector space into the even part of the Clifford algebra over a $(2L+2)$-dimensional vector space, which is related to a global symmetry of the latter algebra (see [22]). We need to stress that the usual Clifford symmetry is not a symmetry of our chain (see [22]), but nonetheless it might be possible to find a symmetry on the chain which is responsible for the 'projection'.

In the thermodynamic limit, the partition function corresponding to the conserved quantity takes on the form of a combinatorial generating function, which is due to the nature of the operator. This raises two sets of questions. What type of properties such as modularity can we infer from the physical description? And on the other hand, what modes or pseudo-particle excitations correspond to the new conserved quantity? We hope that we can shed some light on both of these problems in the future.

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