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The XX-model with boundaries: Part I. Diagonalization of the finite chain

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Abstract. This is the first of three papers dealing with the XX finite quantum chain with arbitrary, not necessarily Hermitian, boundary terms. This extends previous work where the periodic or diagonal boundary terms were considered. In order to find the spectrum and wavefunctions, an auxiliary quantum chain is examined which is quadratic in fermionic creation and annihilation operators and hence diagonalizable. The secular equation is, in general, complicated but several cases were found when it can be solved analytically. For these cases the ground-state energies are given. The appearance of boundary states is also discussed and in view of the applications considered in the next papers, the one- and two-point functions are expressed in terms of Pfaffians.

1. Introduction

In this paper, we consider the XX-chain with diagonal and non-diagonal boundary terms:

$$H = \frac{1}{2}\sum_{j=1}^{L-1}[\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+] + \frac{1}{\sqrt{8}}[\alpha_-\sigma_1^- + \alpha_+\sigma_1^+ + \alpha_z\sigma_1^z + \beta_+\sigma_L^+ + \beta_-\sigma_L^- + \beta_z\sigma_L^z]. \tag{1.1}$$

Here, $\sigma^\pm$ are defined by $\sigma^\pm = \frac{1}{2}(\sigma^x \pm \mathrm{i}\sigma^y)$, where σ^x, σ^y and σ^z are the Pauli matrices. The factor $1/\sqrt{8}$ has been introduced for later convenience. Since the parameters $\alpha_\pm$, $\beta_\pm$, α_z and β_z are arbitrary complex numbers, the Hamiltonian defined by equation (1.1) is non-Hermitian in the general case.

Let us now give a brief overview of the literature before turning to the concrete results we obtained by studying diagonal and non-diagonal boundary conditions. All the articles mentioned in this overview are based on the free-fermion approach to the XX-model.

The XX-model often appears as a special case of the XY-model. The XY-model was introduced 1961 by Lieb *et al* [1] who computed its ground-state energy, the elementary excitations and also presented a method to calculate time-independent correlation functions. In this way, they treated periodic boundary conditions as well as free ends.

During the last 30 years, the correlation functions of the XY-model and therewith the XX-model have been the subject of various investigations. McCoy [2] studied the correlation functions of the XY-model with periodic boundary conditions. More precisely, he computed the asymptotic behaviour of each of the three time-independent correlation functions $\langle\sigma_0^i\sigma_R^i\rangle$ with $i = x, y, z$ in the limit $R \to \infty$. Barouch and McCoy [3] determined the

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asymptotic behaviour of the same correlation functions for the XY-model with an external time-independent magnetic field in the z-direction. In another article, time-dependent spin–spin correlation functions of the form $\langle\sigma_0^x(t)\sigma_R^x(0)\rangle$ and $\langle\sigma_0^y(t)\sigma_R^y(0)\rangle$ for the XY-model in an external magnetic field again in the z-direction were calculated in the limit of large R by McCoy *et al* [4]. Exact expressions for these correlation functions for all values of R and t were then computed by Vaidya and Tracy [5]. Furthermore, time-dependent many-spin correlation functions for the XY-model in an external constant magnetic field in the z-direction were treated by Bariev [6].

Recently, the XY-model with boundary terms has been the subject of increasing interest. Hinrichsen and Rittenberg [7] showed that the anisotropic XY-model in an external magnetic field with σ^z-boundary terms is invariant under certain quantum group transformations. Furthermore, they defined and calculated the corresponding invariant correlation functions.

The XX-model with non-diagonal boundary terms, however, has not been studied thoroughly before. Some work in this direction has been presented by Guinea [8] who studied the semi-infinite XY-model with one σ^x-boundary term (i.e. $\alpha_- = \alpha_+ = 1, \beta_+ = \beta_- = \alpha_z = \beta_z = 0$). We will mention more details of that paper when discussing the physical applications of the Hamiltonian H of equation (1.1). Furthermore, a study of the totally asymmetric XX-model with bulk terms of the form $\sigma_j^+\sigma_{j+1}^-$ and with boundary parameters given by $\alpha_- \neq 0, \beta_+ \neq 0, \alpha_+ = \beta_- = \alpha_z = \beta_z = 0$ in the notation of equation (1.1) can be found in our previous paper [9].

As already mentioned, in the general case the Hamiltonian given by equation (1.1) is non-Hermitian. Interesting physical problems involving non-Hermitian Hamiltonians can be found in several articles treating non-Hermitian quantum mechanics [10].

The Hamiltonian given by equation (1.1) can also be used in the study of asymmetric bulk terms. More precisely, starting from a Hamiltonian of the form

$$\tilde{H} = \sum_{j=1}^{L-1}[p\sigma_j^+\sigma_{j+1}^- + q\sigma_j^-\sigma_{j+1}^+] + \frac{1}{\sqrt{8}}[\alpha'_-\sigma_1^- + \alpha'_+\sigma_1^+ + \alpha_z\sigma_1^z + \beta'_+\sigma_L^+ + \beta'_-\sigma_L^- + \beta_z\sigma_L^z] \tag{1.2}$$

one can use a similarity transformation (see, for example, [11]) that transforms the asymmetric bulk terms depending on the two parameters p and q of the Hamiltonian given by equation (1.2) into symmetric bulk terms. It is convenient to choose $\sqrt{pq} = \frac{1}{2}$. Note that the similarity transformation changes the boundary terms. The corresponding transformed boundary parameters α_-, α_+, β_+ and β_- of the Hamiltonian given by equation (1.1) are now L-dependent and have the expressions

$$\begin{aligned} \alpha_- &= Q^{(1-L)/2}\alpha'_- \qquad & \alpha_+ &= Q^{(L-1)/2}\alpha'_+ \\ \beta_+ &= Q^{(1-L)/2}\beta'_+ \qquad & \beta_- &= Q^{(L-1)/2}\beta'_- \end{aligned} \tag{1.3}$$

with $Q = \sqrt{q/p}$. The diagonal boundary terms remain unchanged.

Although the Hamiltonian of the XYZ-chain with non-diagonal boundary terms is known to be integrable [12, 13], Bethe ansatz equations have not yet been obtained, because it is not clear how to construct a reference state. Therefore, to study the effect of non-diagonal boundary terms, we chose the XX-model with boundaries of the form given by equation (1.1), because this model can be fermionized. To be able to use the free-fermion approach, we introduce a new Hamiltonian H_{long} which is bilinear in terms of fermionic creation and annihilation operators. This approach has the major advantage that we have complete control over the wavefunctions for a large class of boundary parameters which enables us to calculate correlation functions. Thus, we get a good handle on a particularly interesting and important integrable model.

As mentioned above, in order to treat the Hamiltonian given by equation (1.1) we transfer the diagonalization problem to a new Hamiltonian which we obtain by appending one additional site at each end of the chain as in [14]. This new Hamiltonian has the following expression:

$$H_{\rm long} = \frac{1}{2}\sum_{j=1}^{L-1}[\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+] + \frac{1}{\sqrt{8}}[\alpha_-\sigma_0^x\sigma_1^- + \alpha_+\sigma_0^x\sigma_1^+ + \alpha_z\sigma_1^z + \beta_+\sigma_L^+\sigma_{L+1}^x + \beta_-\sigma_L^-\sigma_{L+1}^x + \beta_z\sigma_L^z]. \tag{1.4}$$

In this way, the boundary terms are also bilinear expressions in the σ^+ and σ^- matrices. It is only after this transformation that we can write and solve the problem in terms of free fermions. Since σ_0^x and σ_{L+1}^x commute with $H_{\rm long}$, the spectrum of $H_{\rm long}$ decomposes into four sectors $(++, +-, -+, --)$ corresponding to the eigenvalues ± 1 of σ_0^x and σ_{L+1}^x. The original Hamiltonian corresponds to the $(++)$-sector. A substantial part of this paper is devoted to showing how the eigenvalues of H are obtained by projecting onto this sector.

The Hamiltonian $H_{\rm long}$ which we introduced only as a means to treat the Hamiltonian H is actually interesting in its own right as a quantum spin chain with boundary terms.

In the field-theoretic approach the Hamiltonian $H_{\rm long}$ is probably related to the decoupling point of the boundary sine–Gordon model. The corresponding boundary S-matrix has been calculated in [15, 16].

It is very likely that the Hamiltonian H given by equation (1.1) can be applied to physical problems, since a simpler version of this Hamiltonian has already found such applications. Namely, the semi-infinite XX-chain with one σ^x-boundary term mentioned before was studied by Guinea [8] as a model for the dynamics of a particle in an external potential coupled to a dissipative environment. He also utilized free fermions and presented an explicit solution for the mobility of the particle in the continuum limit. Afterwards this solution was used in the study of transmission through resonant barriers and resonant tunnelling in an interacting one-dimensional electron gas, cf Kane and Fisher [17]. This type of system is studied in experiments with quantum wires. The calculation is built on a perturbative renormalization group analysis in different limits (limits of a weak barrier and a strong barrier). By combining the results of these two limits the authors obtain the full phase diagram of the model. For one particular value of the dimensionless conductance, they even obtain an exact solution for the conductance through a resonance by mapping the model onto the semi-infinite XX-model with one σ^x-boundary term.

The starting point for our investigations of the XX-chain with non-diagonal boundary terms is the diagonalization of the Hamiltonian H (equation (1.1)). This problem is not only of mathematical interest, since the model has an interesting physical content. Namely, as will be shown, boundary bound states appear and the non-trivial ground-state expectation values of the σ_j^x-operators and the σ_j^z-operators exhibit a decay into the bulk which can be predicted from conformal field theory. Furthermore, the expressions for the partition functions formally coincide with partition functions of a Coulomb gas with only magnetic charges or only electric charges, depending on the choice of the boundary parameters in the Hamiltonian H. Additionally, the fermionic energies as well as the expressions for the ground-state energies show a logarithmic dependence on the lattice length for special choices of the boundary parameters. The study of these physical properties is deferred to two subsequent papers. In the following we summarize the content of all the papers and point out how the results of the present paper enter into the further considerations.

In this first paper, we confine ourselves to studying the integrable model with non-diagonal boundary terms given by H on a finite chain. This includes the calculation of the spectrum and the wavefunctions as well as the derivation of expressions for the one-

and two-point correlation functions for the σ_j^x-operators where the subscript j indicates the position on the chain. These results are obtained in parallel for H and H_{long}. Let us briefly describe how we proceed. We start by fermionizing the Hamiltonian H_{long}. The spectrum of the original chain as well as the eigenvectors can be retrieved from the spectrum and the eigenvectors of H_{long} by a projection technique which we derive in detail. As a by-product, we solve the eigenvalue problem for the quantum spin chain H_{long}. We demonstrate that after fermionization the problem of finding the eigenvalues of the Hamiltonian H_{long} is reduced to the problem of finding the zeros of a complex polynomial of degree $2L + 4$, which we write down explicitly. This polynomial, which might very well also appear in other contexts, has interesting algebraical properties. Namely, for some choices of the parameters, it can be factorized into cyclotomic polynomials. We looked systematically for these factorizations since, apart from being of mathematical interest, these examples give access to an exact solution for the full spectrum of the Hamiltonian, including exact expressions for the ground-state energy. (In the general, non-Hermitian case, we define the ground-state energy to be the one with the smallest real part.) Some of these examples are especially interesting since the factorizations contain L-independent factors which lead to L-independent energy gaps of the Hamiltonian. The corresponding eigenstates will be identified as boundary bound states in the next paper. Furthermore, the 'cyclotomic' examples furnish a reliable ansatz for an approximative study of the zeros of the polynomial in the general case which will be presented in the third paper. As an additional result, we get exact formulae for the one- and two-point correlation functions for the σ_j^x-operators. The value of $\langle\sigma_{L+1}^x\rangle$ enters the projection mechanism mentioned above.

In the second paper, by using the results of the first paper, we calculate one-point functions for the σ_j^x- and the σ_j^z-operators for arbitrary position j and lattice length L for several of the 'exactly solvable' cases where the polynomial can be factorized into cyclotomic polynomials. These one-point functions decay into the bulk with a power law typical of conformally invariant theories. Taking this point of view, we determine their critical exponents.

Furthermore, we make the connection between excitations with an L-independent energy seen in this paper and boundary bound states. This identification is made, on the one hand, by studying the spatial profile of the special fermionic excitations in comparison to the spatial profile of other fermionic excitations and, on the other hand, by comparing them to boundary bound states found in the Bethe ansatz for the XXZ-chain with diagonal boundary terms [19]. Boundary bound states originally appeared in the field-theoretic approach to the sine–Gordon model with boundary interaction [12, 16, 18]. In our case, it is surprising that they are related to special zeros of the complex polynomial as mentioned above and can therefore be found without invoking the field theory.

A further important new observation is related to the partition functions in the thermodynamic limit. They will be presented in the third paper, where they will be derived by studying approximative solutions of the polynomial equation for large values of L as mentioned above. The partition functions correspond to conformally invariant systems, a behaviour which we also found in our previous study of the totally asymmetric XX-chain with non-diagonal boundary terms [9]. This observation is confirmed by the expansions of the exactly calculated ground-state energies for large L. From this expansion one can read off the conformal charge $c = 1$ and obtain expressions for the surface free energy. Moreover, the partition functions we find are the partition functions of a Coulomb gas with only magnetic charges or only electric charges. The phenomenon of finding only magnetic charges is elucidated by the construction of a pseudoscalar magnetic charge operator from the fermionic number operators which commutes with the Hamiltonian for finite chains. Furthermore, for special choices of the boundary parameters, we find a logarithmic L-dependence for the fermionic energies as well

as for the expression for the ground-state energies. This may only happen if the Hamiltonian is non-Hermitian.

The present paper is very technical by nature. For those readers who are not interested in all the details of our calculations but would nevertheless like to use our results without reading the whole paper we provide a guide in section 13, which does not, however, follow the sections in a chronological way. The other sections are organized as follows. In section 2, we use the fermionization of the chain H_{long} to reduce the eigenvalue problem of this Hamiltonian to the eigenvalue problem of a matrix M of dimension $(2L+4) \times (2L+4)$ whose eigenvalues correspond to the fermionic energies. We derive some general properties of the eigenvectors of M (which will be needed in sections 10 and 11) before showing, in section 3, how the eigenvectors corresponding to the non-zero eigenvalues of M can be calculated explicitly. The solution of the eigenvalue problem of M leads to a complex polynomial (which corresponds to the characteristic polynomial of M) whose zeros determine all eigenvalues and eigenvectors of M. This polynomial is presented in section 4. Section 5 is devoted to the study of the factorization properties of this polynomial. By constraining the total number of cyclotomic factors, we systematically determined the boundary parameters for which the polynomial factorizes into cyclotomic polynomials. Some of these cases are actually one-parameter families of solutions. In section 6, we show for two examples how the full spectrum of H_{long} is obtained from the factorized form of the polynomial. Section 7 contains the exact expressions for the ground-state energies of all examples where the polynomial factorizes into cyclotomic polynomials. In section 8, we present one example of a Hamiltonian with asymmetric bulk terms where it is also possible to calculate the full spectrum and the ground-state energy exactly for arbitrary values of L. In section 9, we derive the projection mechanism which is needed to obtain the spectrum of the original Hamiltonian from H_{long}. To derive the projection mechanism we need the value of the one-point function of the σ_j^x-operator at the point $j = L+1$. We express the one- and two-point correlation functions of σ_j^x in terms of Pfaffians in section 10. In the cases where the Hamiltonian H has no σ^z boundary terms or fulfils the condition $\alpha_- = \alpha_+$ and $\beta_+ = \beta_-$, we further reduce these Pfaffians to subdeterminants of a certain matrix. These expressions will be needed for the calculation of spatial profiles in our second paper. In section 11, we calculate the above-mentioned value of the one-point function of σ_j^x at the point $j = L+1$ in the cases where the Hamiltonian is: (a) Hermitian, (b) has no σ^z boundary terms or (c) fulfils the condition $\alpha_- = \alpha_+$ and $\beta_+ = \beta_-$. Inputting this result, we invoke the projection mechanism and present the ground-state energies for the original Hamiltonian H in the 'exactly solvable' cases which additionally satisfy at least one of the afore-mentioned conditions (a)–(c) in section 12. We conclude this paper with a discussion of our results in section 14. In an appendix we show how to find the eigenvectors of the matrix M corresponding to the eigenvalue zero. We derive the conditions for the appearance of zero modes in the spectrum of H_{long} and determine respective restrictions for the boundary parameters.

2. Diagonalization of the Hamiltonian

In this section, we present the general formalism we use for the diagonalization of the XX-model with boundary terms defined by equation (1.1). H can be diagonalized in terms of free fermions if it can be written as a bilinear expression in $\sigma^{\pm}$-matrices, since standard fermionization techniques can then be applied [1, 20].

To obtain a bilinear expression in $\sigma^{\pm}$-matrices for H we add one lattice site at each end of the chain, site 0 and site $L+1$ as in [14]. Notice that the terms containing σ^z do not have

to be changed. The Hamiltonian now reads

$$H_{\text{long}} = \frac{1}{2}\sum_{j=1}^{L-1}[\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+] + \frac{1}{\sqrt{8}}[\alpha_-\sigma_0^x\sigma_1^- + \alpha_+\sigma_0^x\sigma_1^+ + \alpha_z\sigma_1^z + \beta_+\sigma_L^+\sigma_{L+1}^x + \beta_-\sigma_L^-\sigma_{L+1}^x + \beta_z\sigma_L^z]. \tag{2.1}$$

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. Notice that the projection of H_{long} onto a fixed sector (ϵ_1, ϵ_2) has the same eigenvalues as the original Hamiltonian with the choice of the parameters $\epsilon_1\alpha_-$, $\epsilon_1\alpha_+$, $\epsilon_2\beta_-$ and $\epsilon_2\beta_+$ so that by diagonalizing H_{long} one simultanously treats four different Hamiltonians H. The eigenvectors of the original choice of the parameters α_-, α_+, β_- and β_+ can be retrieved by projecting onto the $(++)$-sector as described in section 9.

Furthermore, notice that the $(++)$-sector and the $(--)$-sector respectively the $(+-)$-sector and the $(-+)$-sector can be interchanged by using the following transformation which leaves H_{long} invariant:

$$\sigma_j^x \to -\sigma_j^x \qquad \sigma_j^y \to -\sigma_j^y \qquad \sigma_j^z \to \sigma_j^z \qquad j = 0, \ldots, L+1. \tag{2.2}$$

It maps any eigenvector $|\Psi\rangle$ of H_{long} from the (ϵ_1, ϵ_2)-sector onto an eigenvector $|\Psi\rangle'$ of H_{long} with the same eigenvalue lying in the sector $(-\epsilon_1, -\epsilon_2)$. Therefore, each eigenvalue of H_{long} is at least twofold degenerate. In the fermionic language, the above symmetry manifests itself as a zero mode.

In the next section, we will show that the diagonalization of H_{long} can be reduced to finding the eigenvalues and the eigenvectors of a $(2L+4)\times(2L+4)$ matrix which will be denoted by M. After studying general properties of the eigenvectors, we will describe in section 3 how they can be obtained in an explicit form. The eigenvectors and the eigenvalues of the matrix M are determined by the zeros of a polynomial which will be given in section 4.

2.1. Diagonalization of H_{long}

Adopting the Majorana representation of the lattice $s = 1/2$ spin operators as in [21], set

$$\tau_j^{+,-} = \left(\prod_{i=0}^{j-1}\sigma_i^z\right)\sigma_j^{x,y}. \tag{2.3}$$

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

$$H_{\text{long}} = -\sum_{\mu,\nu=\pm1}\sum_{j=1}^{L-1} F^{\mu,\nu}\tau_j^\mu\tau_{j+1}^\nu + G^{\mu,\nu}\tau_0^\mu\tau_1^\nu + K^{\mu,\nu}\tau_L^\mu\tau_{L+1}^\nu + I^{\mu,\nu}\tau_1^\mu\tau_1^\nu + J^{\mu,\nu}\tau_L^\mu\tau_L^\nu \tag{2.4}$$

where

$$G = \frac{1}{2}\begin{pmatrix} \frac{1}{\sqrt{8}}(\alpha_- - \alpha_+) & \frac{1}{\sqrt{8}}\mathrm{i}(\alpha_- + \alpha_+) \\ 0 & 0 \end{pmatrix} \qquad K = \frac{1}{2}\begin{pmatrix} 0 & \frac{1}{\sqrt{8}}\mathrm{i}(\beta_+ + \beta_-) \\ 0 & \frac{1}{\sqrt{8}}(\beta_+ - \beta_-) \end{pmatrix}$$
$$F = \frac{1}{4}\begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix} \qquad I = \frac{1}{2}\begin{pmatrix} 0 & -\frac{1}{\sqrt{8}}\mathrm{i}\alpha_z \\ \frac{1}{\sqrt{8}}\mathrm{i}\alpha_z & 0 \end{pmatrix} \qquad J = \frac{1}{2}\begin{pmatrix} 0 & -\frac{1}{\sqrt{8}}\mathrm{i}\beta_z \\ \frac{1}{\sqrt{8}}\mathrm{i}\beta_z & 0 \end{pmatrix}. \tag{2.5}$$

Here we chose the basis such that the matrices above have the general form

$$A = \begin{pmatrix} A^{--} & A^{-+} \\ A^{+-} & A^{++} \end{pmatrix}$$

where A is one of the matrices in (2.5). Now we apply a linear transformation to the $\tau_j^{+,-}$ operators to obtain another set T_n^+, T_n^- of Clifford operators satisfying

$$\{T_m^\mu, T_n^\nu\} = 2\delta_{nm}^{\mu\nu}. \tag{2.6}$$

Let

$$T_n^\gamma = \sum_{j=0}^{L+1} \sum_{\mu=\pm 1} (\psi_n^\gamma)_j^\mu \tau_j^\mu \tag{2.7}$$

be the explicit form of this linear transformation where $\gamma = \pm 1$. One can choose this linear transformation in such a way that in terms of these new Clifford operators H_{long} takes the simple form

$$H_{\text{long}} = \sum_{n=0}^{L+1} \Lambda_n \mathrm{i} T_n^- T_n^+. \tag{2.8}$$

The commutation relations for the T_n^-, T_n^+ imply that the operator $\mathrm{i}T_n^- T_n^+$ has eigenvalues ± 1 so that the spectrum of H_{long} is given by all possible linear combinations involving all Λ_n with coefficients +1 or -1 and can be read off equation (2.8).

Notice that the operators T_n^-, T_n^+ as defined by equation (2.7) are, in general, non-Hermitian. However, according to a general theorem for Clifford operators [22], it is possible to apply a similarity transformation to the set of vectors (ψ_n^+) and (ψ_n^-) to obtain new Hermitian Clifford operators $T_n^{-\prime}$, $T_n^{+\prime}$ in terms of which the Hamiltonian also takes the form given by equation (2.8). This will be discussed in detail in the next section.

The coefficients $(\psi_n^\gamma)_j^\mu$ of equation (2.7) are constrained by requiring that the operators T_n^γ obey the anticommutation relations of equation (2.6). By computing the commutator $[H_{\text{long}}, T_n^\pm]$ using for H_{long} first the expression (2.8) and then (2.4), and comparing both results, one finds that the eigenvalues Λ_n and the vectors

$$\psi_n^\gamma = ((\psi_n^\gamma)_0^-, (\psi_n^\gamma)_0^+, \ldots, (\psi_n^\gamma)_{L+1}^-, (\psi_n^\gamma)_{L+1}^+) \qquad \gamma = \pm \tag{2.9}$$

are given by the solutions of the following equations

$$M\psi_n^+ = -\mathrm{i}\Lambda_n \psi_n^- \qquad M\psi_n^- = \mathrm{i}\Lambda_n \psi_n^+ \tag{2.10}$$

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

$$M = \begin{pmatrix} 0 & G & & & & \\ -G^T & 2I & F & & & \\ & -F^T & 0 & F & & \\ & & \cdots & \cdots & \cdots & \\ & & & -F^T & 2J & K \\ & & & & -K^T & 0 \end{pmatrix}. \tag{2.11}$$

Defining

$$\phi_n^+ = \psi_n^+ - \mathrm{i}\psi_n^- \qquad \phi_n^- = \psi_n^+ + \mathrm{i}\psi_n^- \tag{2.12}$$

leads to the eigenvalue problem

$$M\phi_n^\pm = \pm\Lambda_n \phi_n^\pm. \tag{2.13}$$

Observe that M has $2L+4$ eigenvalues although H_{long} has only length $L+2$. This can be explained by considering equation (2.13). As one can see, with the appearance of each eigenvalue Λ_n we also get the negative eigenvalue $-\Lambda_n$. As mentioned above, the spectrum of H_{long} is given by all linear combinations of Λ_n with coefficients ± 1 (see (2.8)) and thus can be retrieved from the eigenvalues of M by choosing from each pair of eigenvalues $\pm\Lambda_n$

one value as a basis element for the $\mathbb{Z}_2$–linear combinations. Later we will make this choice in a systematic way following a physical convention which consists of choosing as relevant energies the eigenvalues with positive real part.

As can be seen directly from the form of M, at least two of the eigenvalues are zero. The corresponding eigenvectors are given by $(0, 1, 0, 0, \ldots, 0)$ and $(0, 0, \ldots, 0, 1, 0)$. Since the eigenvalues of M occur in pairs $\pm\Lambda_n$, from which only one value has to be taken, the zero eigenvalues lead to one zero mode as already mentioned above. As we are going to see more explicitly, this zero mode does not appear as a fermionic excitation in the spectrum of H. This fact can be explained as follows. Recall that in the case of H_{long} the zero mode reflects the presence of the symmetry given by equation (2.2) which interchanges the $(++)$-sector and the $(--)$-sector respectively the $(+-)$-sector and the $(-+)$-sector. Since H corresponds only to the $(++)$-sector, it is clear that the above symmetry is not a symmetry of H. Therefore, the above zero mode does not appear in the spectrum of H. In the following we are going to call it the spurious zero mode.

To express the spectrum of H_{long} in terms of free fermions, we will now write the expression for the Hamiltonian in terms of fermionic operators b_n and a_n satisfying

$$\{b_n, a_m\} = \delta_{n,m} \qquad \{b_n, b_m\} = 0 \qquad \{a_n, a_m\} = 0 \tag{2.14}$$

which are obtained from the Clifford operators T_n^+ and T_n^- by the following transformation:

$$b_n = \tfrac{1}{2}(T_n^+ + \mathrm{i}T_n^-) \qquad a_n = \tfrac{1}{2}(T_n^+ - \mathrm{i}T_n^-). \tag{2.15}$$

H_{long} then reads

$$H_{\text{long}} = \sum_{n=0}^{L+1} 2\Lambda_n b_n a_n - \sum_{n=0}^{L+1} \Lambda_n = \sum_{n=0}^{L+1} 2\Lambda_n N_n + E_0 \tag{2.16}$$

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

Notice that in the expression for the number operator N_n in equation (2.16) b_n is equal to $a_n^\dagger$ if the operators T_n^+ and T_n^- are Hermitian. As mentioned above, they can always be chosen to be Hermitian by applying a similarity transformation to the vectors (ψ_n^+) and (ψ_n^-) in equation (2.7). At the same time, the operators a_n and b_n are then transformed into new operators a_n' and b_n' which are adjoints of each other.

In equation (2.16) we have defined the Fermi sea by summing over all negative eigenvalues of M. Consequently, we have to choose the other half of the eigenvalues of M to form fermionic excitations above the Fermi sea. Here and in the following we will use the convention that if a pair of eigenvalues has non-vanishing real part, we will denote that with positive real part by Λ_n. This choice leads to a ground-state energy with the smallest real part. In the case where the real part (but not the imaginary part) of Λ_n is zero, one has the freedom of choice to take either the eigenvalue with positive or the eigenvalue with negative imaginary part as a fermionic excitation above the Fermi sea. This leads to an ambiguity in the value of the imaginary part of the ground-state energy. A similar problem occurs in the calculations involving the eigenvectors of the zero modes (e.g. in the calculation of one-point functions of σ-operators). Namely, the zero eigenvalues of M also occur in pairs ('+0' and '$-$0') and one can freely choose which of these two zero eigenvalues belongs to the Fermi sea and which one corresponds to an excitation with zero energy. In other words, one can choose which is the creation and which the annihilation operator corresponding to the fermion with zero energy. We will come back to this point in [23].

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 (2.7),

$$a_m = \frac{1}{2}(T_m^+ - \mathrm{i}T_m^-) = \frac{1}{2}\sum_{j=0}^{L+1}\sum_{\mu=\pm 1}(\phi_m^+)_j^\mu \tau_j^\mu \tag{2.17}$$

$$b_m = \frac{1}{2}(T_m^+ + \mathrm{i}T_m^-) = \frac{1}{2}\sum_{j=0}^{L+1}\sum_{\mu=\pm 1}(\phi_m^-)_j^\mu \tau_j^\mu. \tag{2.18}$$

Notice that if one transforms the operators T_n^-, T_n^+ into Hermitian operators as mentioned above, the set of vectors (ϕ_m^+), (ϕ_m^-) fulfils the conditions $(\phi_m^+) = (\phi_m^-)^*$ and b_m becomes the adjoint of a_m.

2.2. Orthogonality relations

In the following, we make some general remarks on the given eigenvalue problem for the skew-symmetric matrix $M = -M^t$ defined by equation (2.13). We show that we can indeed find a linear transformation of the form given by equation (2.7) in terms of the vectors $(\psi_n^\gamma)_j^\mu$ (which are related to the eigenvectors of M by equation (2.12)) such that a_k and b_k of equations (2.18) and (2.17) satisfy (2.14) or equivalently that the $T_k^\pm$ of equation (2.7) are Clifford operators respectively, i.e. they satisfy (2.6), which was assumed before deriving the eigenvalue equation. The corresponding orthogonality relations for the eigenvectors of M which are equivalent to the anti-commutation relations for the operators a_k, b_k lead to further relations between the eigenvectors (see (2.40) and (2.42)) for special choices of the boundary parameters. They simplify the computation of correlation functions and are used for projecting to the (++)-sector of H_{long}. This will be the subject of sections 9–11.

Let us first look at the case where the Hamiltonian is Hermitian, i.e. $\alpha_- = \alpha_+^*$, $\beta_- = \beta_+^*$ and $\alpha_z, \beta_z \in \mathbb{R}$. This implies that M has only purely imaginary entries and is also Hermitian. So its eigenvectors can be chosen to form an orthogonal basis with respect to the standard scalar product. Because $M^* = -M$ we have

$$\phi_k^- \propto \phi_k^{+*} \tag{2.19}$$

which can be directly seen by taking the complex conjugate of the equation $M\phi_k^+ = \Lambda_k\phi_k^+$. Thus, after an appropriate normalization of the eigenvectors the orthogonality condition for the eigenbasis is equivalent to the relations which are necessary and sufficient to define a set of fermionic operators (equation (2.14)):

$$\sum_{j=0}^{L+1}\sum_{\gamma}(\phi_l^+)_j^\gamma(\phi_k^-)_j^\gamma = 2\delta_{lk} \tag{2.20}$$

$$\sum_{j=0}^{L+1}\sum_{\gamma}(\phi_l^+)_j^\gamma(\phi_k^+)_j^\gamma = \sum_{j=0}^{L+1}\sum_{\gamma}(\phi_l^-)_j^\gamma(\phi_k^-)_j^\gamma = 0. \tag{2.21}$$

Note that, due to equation (2.19), ϕ_k^- and ϕ_k^+ can always be normalized so that b_k and a_k are mutually adjoint. For any set of constants $c_k \in \mathbb{C}$, $c_k \neq 0$ the vectors $\psi_k^+ = \frac{1}{2}(c_k\phi_k^+ + c_k^{-1}\phi_k^-)$ and $\psi_k^- = \frac{1}{2}\mathrm{i}(c_k\phi_k^+ - c_k^{-1}\phi_k^-)$ satisfy equations (2.10) and the orthogonality relations

$$\sum_{j=0}^{L+1}\sum_{\gamma}(\psi_l^\mu)_j^\gamma(\psi_k^\nu)_j^\gamma = \delta_{lk}^{\mu\nu} \tag{2.22}$$

and thus the $T_n^\pm$ defined in terms of the $(\psi_n^\gamma)_j^\mu$ by equation (2.7) are Clifford operators. If we define $\mathbf{\Psi}$ to be the $(2L+4)\times(2L+4)$ matrix consisting of the $2L+4$ vectors $\psi_k^\pm$, we

may rewrite equation (2.22) as $\mathbf{\Psi}^{\mathrm{t}}\mathbf{\Psi} = \mathbf{1}$. This simply reflects the fact that the automorphism group of the Clifford algebra is the orthogonal group. Note that here $\mathbf{\Psi}$ is not necessarily real. However, due to equation (2.19), $\mathbf{\Psi}$ can always be made real by tuning the parameters c_k. Since $\mathbf{\Psi}^{\mathrm{t}}\mathbf{\Psi} = \mathbf{1}$ implies $\mathbf{\Psi}\mathbf{\Psi}^{\mathrm{t}} = \mathbf{1}$, we also obtain

$$\sum_{k=0}^{L+1}\sum_{\mu}(\psi_k^{\mu})_j^{\gamma}(\psi_k^{\mu})_i^{\nu} = \delta_{ij}^{\gamma\nu} \tag{2.23}$$

or, in terms of the components of the eigenvectors of M,

$$\sum_{k=0}^{L+1}\sum_{\mu}(\phi_k^{\mu})_j^{\gamma}(\phi_k^{-\mu})_i^{\nu} = 2\delta_{ij}^{\gamma\nu}. \tag{2.24}$$

Using these equations it is possible to invert equations (2.7) and (2.18), (2.17), respectively. This is necessary to express the spin operators $\sigma^x, \sigma^y, \sigma^z$ in terms of ladder operators, which is needed for the calculation of correlation functions and of the projection mechanism. We will use this form of the orthogonality relations in the next subsection, in order to derive some further relations between the eigenvectors.

If the Hamiltonian is not necessarily Hermitian but all of the eigenvalues of M are non-degenerate except for the eigenvalue 0 corresponding to the eigenvectors $(0, 1, 0, 0, \ldots)$ and $(0, 0, \ldots, 1, 0)$, one can still show that equations (2.20) and (2.21) remain valid. In general, the argument breaks down because M is not necessarily diagonalizable. This will become apparent in sections 3–5.

Choosing the linear combinations

$$\phi_0^{+} = (0, 1, 0, \ldots, 0, \mathrm{i}, 0) \qquad \phi_0^{-} = (0, 1, 0, \ldots, 0, -\mathrm{i}, 0) \tag{2.25}$$

as the eigenvectors corresponding to the eigenvalue 0, we ensure that they also satisfy equations (2.20) and (2.21). We now check equations (2.20) and (2.21) for the other eigenvectors of M.

First, let ϕ^{+} be a right eigenvector corresponding to the eigenvalue Λ, i.e.

$$M\phi^{+} = \Lambda\phi^{+}. \tag{2.26}$$

Because $M = -M^{\mathrm{t}}$, this eigenvector is also a left eigenvector corresponding to the eigenvalue $-\Lambda$, i.e.

$$\phi^{+\mathrm{t}}M = -\Lambda\phi^{+\mathrm{t}}. \tag{2.27}$$

This implies the existence of a right eigenvector ϕ^{-} corresponding to the eigenvalue $-\Lambda$.

Now let ϕ_k and ϕ_l be eigenvectors corresponding to eigenvalues λ_k and λ_l, where we do not restrict the real parts of λ_k and λ_l to be positive or negative. Using equations (2.26) and (2.27) we get

$$\phi_k{}^{\mathrm{t}}\phi_l = \frac{-\lambda_k}{\lambda_l}\phi_k{}^{\mathrm{t}}\phi_l. \tag{2.28}$$

So all products of the form $\phi_k{}^{\mathrm{t}}\phi_l$ are zero if $\lambda_k \neq -\lambda_l$. This gives equation (2.21).

To proof the validity of equation (2.20) we additionally have to show that in the case $-\lambda_k = \lambda_l$ the product $\phi_k{}^{\mathrm{t}}\phi_l$ cannot vanish. This can be done by considering $\phi_l{}^{\dagger}\phi_l$ which is always different from zero if $\phi_l \neq 0$. Now, due to the assumption of non-degenerate eigenvalues, the eigenvectors form a basis and thus $\phi_l{}^{*}$ can be expressed in terms of eigenvectors ϕ_j. Using equation (2.28) with $-\lambda_k = \lambda_l$ we have

$$0 \neq \phi_l^{\dagger}\phi_l = \phi_l^{*\mathrm{t}}\phi_l = \sum_j a_j\phi_j^{\mathrm{t}}\phi_l = a_k\phi_k^{\mathrm{t}}\phi_l. \tag{2.29}$$

The only term left in the expansion of the product $\phi_l^\dagger \phi_l$ is proportional to the product $\phi_k{}^{\mathrm{t}}\phi_l$ due to equation (2.28) and it therefore cannot vanish. So we can normalize the eigenvectors appropriately in order to satisfy equation (2.20). If there are degeneracies in the spectrum of M, the above proof can be generalized by using the biorthogonality of left and right eigenvectors.

We want to point out that the ladder operators a_k and b_k are not the adjoints of each other in general because relation (2.19) is not valid in general. However, as already mentioned in section 2.1, it is always possible to perform a similarity transformation in order to achieve $b_k^\dagger = a_k$. This can be seen by choosing an arbitrary real symmetric and orthogonal matrix $\mathbf{\Psi}'$. The transformed vectors

$$\psi_k'^{\mu} = \mathbf{\Psi}'\mathbf{\Psi}^{\mathrm{t}}\psi_k^{\mu} \tag{2.30}$$

define a new set of Clifford operators $T_k'^{\pm}$ which are now Hermitian. Hence the operators $b_k' = \frac{1}{2}(T_k'^{+} + \mathrm{i}T_k'^{-})$ and $a_k' = \frac{1}{2}(T_k'^{+} - \mathrm{i}T_k'^{-})$ form a set of fermionic ladder operators satisfying $b_k'^{\dagger} = a_k'$. Since the vectors $\phi_k'^{\pm} = \psi_k'^{+} \mp \mathrm{i}\psi_k'^{-}$ are no longer eigenvectors of M but of the transformed matrix

$$M' = \mathbf{\Psi}'\mathbf{\Psi}^{\mathrm{t}} M \mathbf{\Psi}\mathbf{\Psi}'^{\mathrm{t}} \tag{2.31}$$

the transformation (2.30) corresponds to a similarity transformation of the Hamiltonian H_{long}.

2.3. Special properties of eigenvectors

In some cases there are further relations between the eigenvectors in addition to those of equations (2.20) and (2.21). They are used in the calculation of correlation functions and are even necessary for the projection method. First, notice that if $\alpha_z = \beta_z = 0$, the matrices M and M^2 respectively take the form

$$M = \begin{pmatrix} 0 & * & 0 & * & \cdots \\ * & 0 & * & 0 & \\ 0 & * & 0 & * & \\ * & 0 & * & 0 & \\ \vdots & & & & \ddots \end{pmatrix} \qquad M^2 = \begin{pmatrix} * & 0 & * & 0 & \cdots \\ 0 & * & 0 & * & \\ * & 0 & * & 0 & \\ 0 & * & 0 & * & \\ \vdots & & & & \ddots \end{pmatrix} \tag{2.32}$$

where $*$ and 0 both denote 2×2 matrices. Note that $*$ is the notation for an arbitrary 2×2 matrix and is not necessarily different from zero. Looking at equation (2.32) we see that we can choose an eigenvector $\tilde{\psi}_k^+$ of M^2 with eigenvalue Λ_k^2, i.e.

$$M^2\tilde{\psi}_k^+ = \Lambda_k^2\tilde{\psi}_k^+ \tag{2.33}$$

which satisfies

$$(\tilde{\psi}_k^+)_i^{\pm} = 0 \qquad \text{for } i \text{ odd.} \tag{2.34}$$

Now we define $\tilde{\psi}_k^-$ by

$$M\tilde{\psi}_k^+ = -\mathrm{i}\Lambda_k\tilde{\psi}_k^- \tag{2.35}$$

which is also an eigenvector of M^2 with eigenvalue Λ_k^2. Note that this definition does not work if $\Lambda_k = 0$ and thus we have to exclude $k = 0$ in the following, which labels the eigenvectors corresponding to the spurious zero mode. Using equations (2.32) and (2.34) we obtain

$$(\tilde{\psi}_k^-)_i^{\pm} = 0 \qquad \text{for i even.} \tag{2.36}$$

Due to equations (2.33) and (2.35), $\tilde{\psi}_k^+$ and $\tilde{\psi}_k^-$ also satisfy (2.10) and thus we obtain eigenvectors $\tilde{\psi}_k^{\pm} = \tilde{\psi}_k^+ \mp \mathrm{i}\tilde{\psi}_k^-$ of M satisfying

$$(\tilde{\psi}_k^+)_j^{\mu} = (-1)^j(\tilde{\psi}_k^-)_j^{\mu}. \tag{2.37}$$

Therefore, for each pair of vectors ϕ_k^+, ϕ_k^- satisfying equation (2.20), there exists a constant $c \in \mathbb{C}$ such that

$$(\phi_k^+)_j^\mu = c(-1)^j (\phi_k^-)_j^\mu. \tag{2.38}$$

Now equation (2.24) can be rewritten as

$$(1 + (-1)^{i+j}) \sum_{k=0}^{L+1} (\phi_k^+)_j^\gamma (\phi_k^-)_i^\nu = 2\delta_{ij}^{\gamma\nu} \tag{2.39}$$

and we end up with

$$\sum_{k=0}^{L+1} (\phi_k^+)_j^\gamma (\phi_k^-)_i^\nu = \delta_{ij}^{\gamma\nu} \qquad \text{for } i + j \text{ even.} \tag{2.40}$$

Since equation (2.38) is not valid for $k = 0$ and odd L (see (2.25)) we exclude $i = 0, \nu = +, j = L + 1, \gamma = -$ and $j = 0, \gamma = +, i = L + 1, \nu = -$ in equations (2.39) and (2.40).

If diagonal boundary terms are included and if $\alpha_- = \alpha_+$ and $\beta_- = \beta_+$, the eigenvectors again have a special property. In this case M and M^2 also have the form of equation (2.32), but now $*$ and 0 just denote complex numbers and, in place of (2.38), we obtain

$$(\phi_k^+)_j^\pm = \pm c' (\phi_k^-)_j^\pm \tag{2.41}$$

which gives

$$\sum_{k=0}^{L+1} (\phi_k^-)_i^\mu (\phi_k^+)_j^\mu = \delta_{ij}. \tag{2.42}$$

Both equations (2.40) and (2.42) will be used sections 10 and 11.

Note that the proof of (2.40) and (2.42) shown above is not valid if there are degeneracies or zero modes on top of the spurious zero mode in the spectrum of M. However, one can show that it is always possible to build appropriate linear combinations of the eigenvectors corrsponding to the same eigenvalue such that (2.40) and (2.42) remain valid in addition to (2.20) and (2.21). This is not automatically true and, therefore, in explicit calculations one should take care in choosing the right linear combination of eigenvectors corresponding to the degenerate eigenvalues.

If both conditions $\alpha_- = \alpha_+, \beta_- = \beta_+$ and $\alpha_z = \beta_z = 0$ are satisfied at the same time, then both equations (2.40) and (2.42) can be satisfied simultaneously. By comparing (2.38) and (2.41) we obtain the following relation:

$$(\phi_k^-)_j^\pm = \begin{cases} \pm \dfrac{c'}{c} (\phi_k^-)_j^\pm & \text{for } j \text{ even} \\ \mp \dfrac{c'}{c} (\phi_k^-)_j^\pm & \text{for } j \text{ odd.} \end{cases} \tag{2.43}$$

Thus c'/c is either 1 or -1 because otherwise the vectors $\phi_k^\pm$ would vanish.

Let us briefly summarize what we have obtained so far. If H is Hermitian, the fact that $M = -M^{\mathrm{t}}$ leads to equations (2.20) and (2.21) which are equivalent to the anticommutation relations (2.14) of the ladder operators given by (2.18) and (2.17). These equations are still valid if H is non-Hermitian, but diagonalizable. Some additional properties of the eigenvectors have been derived for special choices of the boundary parameters (equation (2.40) for $\alpha_z = \beta_z = 0$ and (2.42) for $\alpha_- = \alpha_+, \beta_- = \beta_+$) which will be used in sections 10 and 11.

3. Calculation of the eigenvectors of the matrix M

In the previous section we have shown some general properties of the eigenvectors without computing them explicitly. This computation is the subject of this section. We will also show how to obtain the characteristic polynomial which gives the eigenvalues of M. This polynomial will be treated extensively in the following sections. Since M is non-Hermitian in general, we will also discuss the diagonalizability of M.

The eigenvalue problem given by equation (2.13) is equivalent to a set of recurrence relations. Using the notation given by equations (2.12) and (2.9) for the eigenvectors $(\phi_k^{\pm})$ of M let us first look at the bulk part:

$$\begin{aligned} &\tfrac{1}{4}\mathrm{i}((\phi_k^{\pm})_j^+ + (\phi_k^{\pm})_{j+2}^+) = \pm\Lambda_k(\phi_k^{\pm})_{j+1}^- \\ &-\tfrac{1}{4}\mathrm{i}((\phi_k^{\pm})_j^- + (\phi_k^{\pm})_{j+2}^-) = \pm\Lambda_k(\phi_k^{\pm})_{j+1}^+ \end{aligned} \qquad (1 \leqslant j \leqslant L-2). \tag{3.1}$$

These bulk equations (3.1) can be decoupled by defining

$$\varphi_j = (\phi_k^{\pm})_j^- + \mathrm{i}(\phi_k^{\pm})_j^+ \qquad \bar{\varphi}_j = (\phi_k^{\pm})_j^- - \mathrm{i}(\phi_k^{\pm})_j^+ \tag{3.2}$$

which gives

$$\tfrac{1}{4}(\varphi_j + \varphi_{j+2}) = \lambda\varphi_{j+1} \qquad -\tfrac{1}{4}(\bar{\varphi}_j + \bar{\varphi}_{j+2}) = \lambda\bar{\varphi}_{j+1}. \tag{3.3}$$

Here $\lambda = \pm\Lambda_k$ and the functions φ_j and $\bar{\varphi}_j$ refer to $(\phi_k^+)_j^-$ and $(\phi_k^+)_j^+$ for $\lambda = \Lambda_k$ and to $(\phi_k^-)_j^-$ and $(\phi_k^-)_j^+$ for $\lambda = -\Lambda_k$. From now on we will keep k fixed and omit all subscripts referring to k.

Next we treat the left boundary and one obtains

$$\begin{aligned} &\varphi_0 = \bar{\varphi}_0 \\ &\lambda\varphi_0 = \tfrac{1}{\sqrt{32}}(\alpha_-\varphi_1 - \alpha_+\bar{\varphi}_1) \end{aligned} \tag{3.4}$$

$$\begin{aligned} &\lambda\varphi_1 = \tfrac{1}{\sqrt{8}}(\alpha_+\varphi_0 - \alpha_z\varphi_1) + \tfrac{1}{4}\varphi_2 \\ &\lambda\bar{\varphi}_1 = \tfrac{1}{\sqrt{8}}(\alpha_z\bar{\varphi}_1 - \alpha_-\bar{\varphi}_0) - \tfrac{1}{4}\bar{\varphi}_2. \end{aligned} \tag{3.5}$$

From the right boundary one gets

$$\begin{aligned} &\lambda\varphi_L = \tfrac{1}{\sqrt{8}}(\beta_+\varphi_{L+1} - \beta_z\varphi_L) + \tfrac{1}{4}\varphi_{L-1} \\ &\lambda\bar{\varphi}_L = \tfrac{1}{\sqrt{8}}(\beta_z\bar{\varphi}_L - \beta_-\bar{\varphi}_{L+1}) - \tfrac{1}{4}\bar{\varphi}_{L-1} \end{aligned} \tag{3.6}$$

$$\begin{aligned} &\lambda\varphi_{L+1} = \tfrac{1}{\sqrt{32}}(\beta_+\bar{\varphi}_L + \beta_-\varphi_L) \\ &\varphi_{L+1} = -\bar{\varphi}_{L+1}. \end{aligned} \tag{3.7}$$

Note that we have excluded explicitly the eigenvectors $(0, 1, 0, \ldots)$ and $(\ldots, 0, 1, 0)$, which always exist, from the set of solutions of the boundary equations above by setting $\varphi_0 = \bar{\varphi}_0$ and $\bar{\varphi}_{L+1} = -\bar{\varphi}_{L+1}$. Thus we will obtain at most $2L + 2$ linearly independent solutions instead of $2L + 4$.

The general solution of the bulk equations (3.3) for $\lambda \neq \pm\frac{1}{2}$ is given by

$$\varphi_j = ax^j + bx^{-j} \qquad \bar{\varphi}_j = g(-x)^j + f(-x)^{-j} \tag{3.8}$$

where $1 \leqslant j \leqslant L$ and up to now a, b, g, f are free parameters which are independent of j. The new variable x is related to the eigenvalue λ via

$$\lambda = \tfrac{1}{4}(x + x^{-1}). \tag{3.9}$$

For $\lambda = \pm\frac{1}{2}$ the general solution is

$$\varphi_j = a(\pm 1)^j + b(\pm 1)^j j \qquad \bar{\varphi}_j = g(\mp 1)^j + f(\mp 1)^j j. \tag{3.10}$$

The four parameters a, b, g, f, the undetermined components $\varphi_0, \bar{\varphi}_0, \varphi_{L+1}, \bar{\varphi}_{L+1}$ and the eigenvalues λ are all fixed by the boundary equations (3.4)–(3.7)—up to the normalization constants of the eigenvectors. Namely, plugging equation (3.8) into (3.4)–(3.7), we obtain a homogeneous system of eight linear equations with the unknowns a, b, g, f and $\varphi_0, \bar{\varphi}_0, \varphi_{L+1}, \bar{\varphi}_{L+1}$. The condition for the existence of non-trivial solutions of this system is given by the vanishing of the determinant of the corresponding 8×8 matrix. This defines a polynomial equation in the variable x which yields all eigenvalues λ. Note that for $x = \pm 1$ the 8×8 system of equations always has the non-trivial solution $a = -b,\ g = -f$. This corresponds to the zero vector $\varphi_j = \bar{\varphi}_j = 0\ \forall j$. To compensate for this fact we divide the polynomial by $(1-x^2)^2$. The treatment of the resulting polynomial equation will be the subject of the next section (see (4.1)).

In the following we will show how to obtain the eigenvectors for $\lambda \neq \pm\frac{1}{2}$ and $\lambda \neq 0$ which may be viewed as an alternative way to obtain the secular equation. Substituting (3.4) into (3.5) using the identity $a = \varphi_1 x^{-1} - b x^{-2}$ and $g = -\bar{\varphi}_1 x^{-1} - f x^{-2}$ (see (3.8)) renders b and f as functions of φ_1 and $\bar{\varphi}_1$, i.e.

$$b = \frac{1}{1-x^{-2}}\left[\left(\frac{\alpha_-\alpha_+}{x+x^{-1}} - \sqrt{2}\alpha_z - x^{-1}\right)\varphi_1 - \frac{\alpha_+^2}{x+x^{-1}}\bar{\varphi}_1\right] \tag{3.11}$$

$$f = \frac{1}{x^{-2}-1}\left[\left(\frac{\alpha_-\alpha_+}{x+x^{-1}} + \sqrt{2}\alpha_z - x^{-1}\right)\bar{\varphi}_1 - \frac{\alpha_-^2}{x+x^{-1}}\varphi_1\right]. \tag{3.12}$$

Thus a and g are given by

$$a = \frac{1}{1-x^2}\left[\left(\frac{\alpha_-\alpha_+}{x+x^{-1}} - \sqrt{2}\alpha_z - x\right)\varphi_1 - \frac{\alpha_+^2}{x+x^{-1}}\bar{\varphi}_1\right] \tag{3.13}$$

$$g = \frac{1}{x^2-1}\left[\left(\frac{\alpha_-\alpha_+}{x+x^{-1}} + \sqrt{2}\alpha_z - x\right)\bar{\varphi}_1 - \frac{\alpha_-^2}{x+x^{-1}}\varphi_1\right]. \tag{3.14}$$

From the right boundary, by substituting (3.7) into (3.6), we see that furthermore

$$\varphi_{L-1} + \left(\frac{\beta_-\beta_+}{4\lambda} - \sqrt{2}\beta_z - 4\lambda\right)\varphi_L + \frac{\beta_+^2}{4\lambda}\bar{\varphi}_L = 0 \tag{3.15}$$

$$\bar{\varphi}_{L-1} - \left(\frac{\beta_-\beta_+}{4\lambda} + \sqrt{2}\beta_z - 4\lambda\right)\bar{\varphi}_L - \frac{\beta_-^2}{4\lambda}\varphi_L = 0. \tag{3.16}$$

Using equations (3.11)–(3.14) and (3.8) in equations (3.15) and (3.16) we get a linear system of equations of the form

$$\begin{pmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{21} & \Omega_{22} \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \bar{\varphi}_1 \end{pmatrix} = 0 \tag{3.17}$$

where Ω_{ij} are the following functions of x and the six boundary parameters $\alpha_\pm$, $\beta_\pm$, α_z and β_z (note that λ is a function of x according to (3.9)):

$$\begin{aligned}\Omega_{11} = {} & \frac{x^{-L}}{1-x^{-2}}\left[\left(\frac{\beta_-\beta_+}{4\lambda} - \sqrt{2}\beta_z - x^{-1}\right)\left(\frac{\alpha_-\alpha_+}{4\lambda} - \sqrt{2}\alpha_z - x^{-1}\right) + (-1)^L\frac{(\beta_+\alpha_-)^2}{4\lambda^2}\right] \\ & + \frac{x^L}{1-x^2}\left[\left(\frac{\beta_-\beta_+}{4\lambda} - \sqrt{2}\beta_z - x\right)\left(\frac{\alpha_-\alpha_+}{4\lambda} - \sqrt{2}\alpha_z - x\right) + (-1)^L\frac{(\beta_+\alpha_-)^2}{16\lambda^2}\right]\end{aligned} \tag{3.18}$$

$$\Omega_{12} = \frac{x^{-L}}{x^{-2}-1}\left[\left(\frac{\beta_-\beta_+}{4\lambda} - \sqrt{2}\beta_z - x^{-1}\right)\frac{\alpha_+^2}{4\lambda} + (-1)^L\left(\frac{\alpha_-\alpha_+}{4\lambda} + \sqrt{2}\alpha_z - x^{-1}\right)\frac{\beta_+^2}{4\lambda}\right] + \frac{x^L}{x^2-1}\left[\left(\frac{\beta_-\beta_+}{4\lambda} - \sqrt{2}\beta_z - x\right)\frac{\alpha_+^2}{4\lambda} + (-1)^L\left(\frac{\alpha_-\alpha_+}{4\lambda} + \sqrt{2}\alpha_z - x\right)\frac{\beta_+^2}{4\lambda}\right] \tag{3.19}$$

$$\Omega_{21} = \frac{x^{-L}}{1-x^{-2}}\left[\left(\frac{\alpha_-\alpha_+}{4\lambda} - \sqrt{2}\alpha_z - x^{-1}\right)\frac{\beta_-^2}{4\lambda} + (-1)^L\left(\frac{\beta_-\beta_+}{4\lambda} + \sqrt{2}\beta_z - x^{-1}\right)\frac{\alpha_-^2}{4\lambda}\right] + \frac{x^L}{1-x^2}\left[\left(\frac{\alpha_-\alpha_+}{4\lambda} - \sqrt{2}\alpha_z - x\right)\frac{\beta_-^2}{4\lambda} + (-1)^L\left(\frac{\beta_-\beta_+}{4\lambda} + \sqrt{2}\beta_z - x\right)\frac{\alpha_-^2}{4\lambda}\right] \tag{3.20}$$

$$\Omega_{22} = \frac{x^{-L}}{x^{-2}-1}\left[\frac{(\alpha_+\beta_-)^2}{16\lambda^2} + (-1)^L\left(\frac{\beta_-\beta_+}{4\lambda} + \sqrt{2}\beta_z - x^{-1}\right)\left(\frac{\alpha_-\alpha_+}{4\lambda} + \sqrt{2}\alpha_z - x^{-1}\right)\right] + \frac{x^L}{x^2-1}\left[\frac{(\alpha_+\beta_-)^2}{16\lambda^2} + (-1)^L\left(\frac{\beta_-\beta_+}{4\lambda} + \sqrt{2}\beta_z - x\right)\left(\frac{\alpha_-\alpha_+}{4\lambda} + \sqrt{2}\alpha_z - x\right)\right]. \tag{3.21}$$

The necessary condition to have non-trivial solutions is obviously that the determinant of the homogeneous equation (3.17) vanishes.

$$\Omega_{11}\Omega_{22} - \Omega_{12}\Omega_{21} = 0. \tag{3.22}$$

This condition is equivalent to the polynomial equation which is obtained from the homogeneous 8×8 system of linear equations mentioned above.

The construction of eigenvectors shown here is not valid for $\lambda = \pm\frac{1}{2}$ and $\lambda = 0$. However, one can show that the eigenvectors for $\lambda = \pm\frac{1}{2}$ can be obtained by

$$\varphi_j = \lim_{x\to\pm1}(ax^j + bx^{-j}) \qquad \bar{\varphi}_j = \lim_{x\to\pm1}(g(-x)^j + f(-x)^{-j}) \tag{3.23}$$

where a, b, g, f are given by equations (3.11)–(3.14). Using de L'Hospital's rule one recovers the form of equation (3.10). The vector components φ_1 and $\bar{\varphi}_1$ are again given as solutions of the 2×2 system (3.17) using $x = \pm1$.

The solution of the 2×2 linear system (3.17) is straightforward for a given set of boundary parameters and a given value of x. It cannot be given in a unique form because some of the Ω_{ij} might vanish. We will give the explicit form of the eigenvectors for some special choices of boundary parameters in [23] where we are going to calculate the expectation values of σ_j^z and σ_j^x where j denotes the position on the lattice.

If all Ω_{ij} vanish the corresponding eigenvalue is at least twofold degenerate and we obtain two linearly independent eigenvectors, since φ_1 and $\bar{\varphi}_1$ can be chosen independently of each other. On the other hand, if a zero of the polynomial is twofold degenerate, it is not clear that all Ω_{ij} vanish. This comes from the fact that the Hamiltonian is in general non-Hermitian and might be non-diagonalizable.

We would like to point out that the appearance of an eigenvalue $\lambda \neq 0$ which is more than twofold degenerate would prove that M is non-diagonalizable. This is indeed the case for some special choices of the boundaries for a given lattice length L. This can be seen by looking at the factorizations of the polynomial obtained in section 5.

Up to now we have shown how to construct the eigenvectors of the matrix M defined by equation (2.11). For $\lambda \neq 0$ the components of the eigenvectors are given by

$$(\phi_k^{\pm})_j^- = \tfrac{1}{2}(\varphi_j + \bar{\varphi}_j) \qquad (\phi_k^{\pm})_j^+ = -\tfrac{1}{2}\mathrm{i}(\varphi_j - \bar{\varphi}_j) \tag{3.24}$$

where φ_j and $\bar{\varphi}_j$ have the form of equation (3.8) for $\lambda \neq \pm\frac{1}{2}$ and are given by (3.23) for $\lambda = \pm\frac{1}{2}$. The parameters a, b, g and f are given by equations (3.11)–(3.14). Finally, λ has to be determined from equation (3.22) as a function of x (see (3.9)). The vanishing of the determinant in equation (3.22) leads to a complex polynomial of degree $4L + 4$ in the variable x which has to be zero. This polynomial will be the subject of the next section.

To obtain eigenvectors corresponding to $\lambda = 0$ one has to solve the boundary equations (3.4)–(3.7) using the bulk solution given by (3.8) with $x = \pm\mathrm{i}$. The calculation is given in the appendix. It turns out that besides the eigenvectors $(0, 1, 0, \ldots)$ and $(\ldots, 0, 1, 0)$ of M, which are always present, one may have additional eigenvectors for $\lambda = 0$. Running through the calculation it turns out that this happens if $\alpha_-\beta_+ + \alpha_+\beta_- = 0$. Under this condition two further linearly independent solutions always exist. If all relevant boundary parameters vanish, i.e. $\alpha_- = \alpha_+ = \beta_- = \beta_+ = 0$, and if at the same time $\alpha_z = -\beta_z$ for L odd or $\alpha_z = 1/2\beta_z$ for L even we have four additional solutions. Two of them are just $(1, 0, 0, \ldots)$ and $(\ldots, 0, 0, 1)$. Note that the degeneracy of the eigenvalue $\lambda = 0$ might be higher than the number of linearly independent eigenvectors since M might be non-diagonalizable. This will be discussed in the appendix by considering the polynomial equation which is given in the next section.

The calculations we have done so far enable us to give a complete set of conditions under which M is non-diagonalizable. This is always the case if the degeneracy of an eigenvalue is higher than the number of linearly independent eigenvectors. The conditions for the eigenvalue $\lambda = 0$ are derived in the appendix, whereas the conditions for the eigenvalues $\lambda \neq 0$ are obtained from equation (3.17). M is non-diagonalizable, if one of the following conditions is satisfied:

(i) M has an eigenvalue $\lambda \neq 0$ which is more than twofold degenerate;

(ii) M has an eigenvalue $\lambda \neq 0$ which is twofold degenerate, but at least one of the Ω_{ij} is different from zero;

(iii) $\lambda = 0$ is an eigenvalue of M, but it is more than sixfold degenerate;

(iv) $\lambda = 0$ is a sixfold degenerate eigenvalue of M, but one of the parameters $\alpha_+, \alpha_-, \beta_+, \beta_-$ is different from zero;

(v) $\lambda = 0$ is a sixfold degenerate eigenvalue of M, but $\alpha_z \neq -\beta_z$ for L odd or $\alpha_z \neq 1/2\beta_z$ for L even, respectively.

If none of these conditions is satisfied, M is diagonalizable.

4. The polynomial equation

Now we turn to the polynomial equation which determines the eigenvalues of M. As can be seen directly from M (equation (2.11)), two of the eigenvalues are always zero. The others are obtained from (3.9), where the values of x are given by the solutions of the following polynomial which has been obtained from (3.22). For later convenience, we use a new variable $z = x^2$:

$$\begin{aligned} p(z) = \frac{1}{(z-1)^2}\Big[& z^{2L+4} - A(z^{2L+3} + z) + (B + E^2)(z^{2L+2} + z^2) \\ & + (D + 2E^2)(z^{2L+1} + z^3) + E^2(z^{2L} + z^4) - 2E(z^{L+4} + z^L) \\ & + \left(\frac{1}{2}(-1 + A - B - D) - (-1)^L C - 2E^2\right)(z^{L+3} + z^{L+1}) \\ & + (-1 + A - B - D + 2(-1)^L C + 4E - 4E^2)z^{L+2} + 1\Big] \end{aligned}$$

$$= \frac{1}{(z-1)^2} q(z) = 0. \tag{4.1}$$

The coefficients are given by

$$\begin{aligned} A &= 2(-1 + \alpha_- \alpha_+ + \beta_+ \beta_- + \alpha_z^2 + \beta_z^2) \\ B &= (-1 + 2\alpha_- g)(-1 + 2\beta_+ \beta_-) + 4(-1 + \alpha_- g)\beta_z^2 + 4(-1 + \beta_+ \beta_-)\alpha_z^2 \\ C &= (\alpha_-^2 \beta_+^2 + \alpha_+^2 \beta_-^2) \\ D &= 2(-1 + 2\alpha_- g)\beta_z^2 + 2(-1 + 2\beta_+ \beta_-)\alpha_z^2 \\ E &= 2\alpha_z \beta_z. \end{aligned} \tag{4.2}$$

Note that the polynomial $p(z)$ is already completely determined by five complex parameters although we started with six parameters in the original Hamiltonian. This can be explained by the existence of a similarity transformation of the form

$$H' = UHU^{-1} \qquad \text{with } U = \prod_{j=1}^{L} I_1 \otimes \cdots \otimes I_{j-1} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \epsilon \end{pmatrix} \otimes I_{j+1} \otimes \cdots \otimes I_L \tag{4.3}$$

containing one free parameter ϵ. Here I_j stands for the identity matrix at the site j. By using this similarity transformation, the four boundary parameters α_-, α_+, β_- and β_+ are transformed as follows

$$\alpha_- \to \epsilon \alpha_- \qquad \alpha_+ \to 1/\epsilon \alpha_+ \qquad \beta_- \to \epsilon \beta_- \qquad \beta_+ \to 1/\epsilon \beta_+ \tag{4.4}$$

and by choosing a particular value of ϵ, one can always fix one of the boundary parameters.

The polynomial $q(z)$ has a very special form, because in comparison with a general polynomial of degree $2L + 4$ many of the coefficients are zero. This changes of course when it is divided by $(z-1)^2$.

Observe that the polynomial $p(z)$ has degree $2L + 2$ although the diagonal form of H_{long} given by equation (2.16) has only $L + 2$ fermionic excitations Λ_n. The reason, therefore, is the quadratic relation between z and Λ. Since with z also $1/z$ is a solution of the polynomial, one gets each value of Λ twice. Taking half of them and adding the additional eigenvalue 0, which was mentioned in section 2 and explicitly excluded from the set of solutions in section 3, gives exactly the $L + 2$ fermionic excitations.

Special solutions of this polynomial will be studied in the next section.

5. Factorization of the polynomial in cyclotomic polynomials

The study of the factorization properties of the polynomial given by equation (4.1) represents a very interesting mathematical problem. Furthermore, factorizations of the polynomial into cyclotomic polynomials which we are going to present below are very important because they allow us to calculate the whole spectrum and other properties of H_{long} analytically.

For some special choices of the parameters A, B, C, D and E the polynomial factorizes exactly into cyclotomic polynomials. These factorizations were found using the following algorithm. A factorized polynomial of degree $2L + 4$ of the form

$$f(z) = \left[\prod_{i=1}^{k} (1 - p_i z^{n_i}) \right] (1 - p_{k+1} z^{2L+4-\sum n_i}) \tag{5.1}$$

is expanded for a fixed value of k (corresponding to a fixed number of factors), a fixed value of L and for all possible combinations of n_i. The coefficients of the expanded polynomial $f(z)$ which are functions of the p_i, $i = 1, \ldots, k + 1$, are compared to the coefficients of the

original polynomial $q(z)$. In this way, one obtains a set of $2L+4$ coupled equations for p_i and the coefficients A, B, C, D and E which has been solved using *Maple*. Typically, values of $L = 5, 6, 7$ were used; for smaller values of L the equations do not reflect the general situation because some exponents coincide. For larger L, however, the number of partitions of $2L + 4$ into n_i, $i = 1, \ldots, k$, becomes too large. Among the solutions only those were kept which are valid for arbitrary L and not only for the special L used in the calculation. k has been varied between 1 and 4. For $k = 5$ (six factors) the program did not run properly—it needed too much memory. However, $q(z)$ cannot factorize into a a larger number of factors of the above form (5.1) than six with the condition that the corresponding n_i appear explicitly as exponents in $q(z)$. In this case the only possible combination for n_i would be

$$n_1 = n_2 = L \qquad n_3 = n_4 = n_5 = n_6 = 1. \tag{5.2}$$

In table 1 all factorizations which were calculated as described above are listed. The factorizations in six factors (entries 14–16) were found by solving the system of coupled equations for the choice (5.2) of n_i and various choices of p_i. Therefore the list might not be exhaustive for the factorizations into six factors.

The entries 10–16 each furnish a one-parameter family of solutions (where the parameter is called s) for which a factorization in cyclotomic polynomials appears. Notice, however, that E is the only parameter whose value is always fixed, independently of s. Since $E = \alpha_z \beta_z$, this means that in all cases presented in table 1 the product of the coefficients in front of the diagonal boundary terms is always fixed. Moreover, the entries 10–16 provide examples where some of the zeros of the polynomial $q(z)$ are always independent of L (e.g. $z = s$ or $z = 1/s$). We will come back to this point in section 7 and in the discussion (section 14).

Looking at the entries 10–16 the remark we made at the end of section 3 that in special cases the Hamiltonian might not be diagonalizable becomes clear: it is possible to choose the parameter s as a function of L in such a way that the polynomial has zeros which are more than twofold degenerate. Take, for example, the case 13 and choose s equal to one solution of $1 - z^L = 0$. Then the corresponding zero of $q(z)$ is threefold degenerate for the value of L chosen above. In this case, one cannot find more than two independent eigenvectors for M (cf (3.17)) for the corresponding degenerate eigenvalue. Thus, in these special cases (which can be constructed analogously for the other entries 10–16) the matrix M is not diagonalizable.

For all examples in table 1 it is possible to calculate the spectrum and the ground-state energy exactly. In the following sections we will give the explicit expressions for the ground-state energies and for some excitations. With the insight gained from these exactly solvable cases we will later also treat the general case in the limit of large L [23].

6. Examples of exact calculations of spectra for the finite lattice

Let us now present two examples of how to calculate the spectrum of H_{long} from the factorized form of the polynomial. We will first take case 4 from table 1. The factorized form of the polynomial $q(z)$ as given in table 1 suggests the ansatz $z = \exp(\mathrm{i}\pi + (2\mathrm{i}\phi/(2L + 1)))$. This leads to the solutions

$$\phi = n\pi \qquad n = 1, \ldots, L. \tag{6.1}$$

The factor $(1 + z)$ leads to the additional solution $z = -1$ which means $\Lambda = 0$. The factor $(1 - z)^2$ has to be divided out because the fermionic energies are given by the zeros of $p(z)$ and not of those of $q(z)$ which are given in table 1 (also cf (4.1)).

Table 1. Cases where the polynomial factorizes into cyclotomic polynomials.

Case	A	B	$(-1)^L C$	D	E	$q(z)$
1	1	0	0	0	0	$(1-z)(1-z^{2L+3})$
2	0	-1	0	0	0	$(1-z^2)(1-z^{2L+2})$
3	-1	0	0	0	0	$(1+z)(1-z^{L+1})(1-z^{L+2})$
4	1	-1	0	1	0	$(1+z)(1-z)^2(1+z^{2L+1})$
5	0	0	$\frac{1}{2}$	0	0	$(1-z^{L+1})(1-z^{L+3})$
6	0	0	$-\frac{1}{2}$	0	0	$(1-z^{L+2})^2$
7	1	0	1	0	0	$(1-z)(1-z^{L+1})(1+z^{L+2})$
8	1	0	-1	0	0	$(1-z)(1+z^{L+1})(1-z^{L+2})$
9	2	1	$s+1/s$	0	0	$(1-z)^2(1-sz^{L+1})(1-1/sz^{L+1})$
10	$s+1/s$	1	$\frac{1}{2}(2+s+1/s)$	0	0	$(1-sz)(1-1/sz)(1-z^{L+1})^2$
11	$1+s+1/s$	$1+s+1/s$	0	-1	0	$(1-sz)(1-1/sz)(1-z)(1-z^{2L+1})$
12	0	$-1-s-1/s$	$\frac{1}{2}(-2+s+1/s)$	-2	1	$(1-sz^2)(1-1/sz^2)(1-z^L)^2$
13	$s+1/s$	1	$-2-s-1/s$	$-2-s-1/s$	1	$(1-sz)(1-1/sz)(1+z^2)(1-z^L)^2$
14	$2+s+1/s$	$1+2s+2/s$	$4+2s+2/s$	$-4-s-1/s$	-1	$(1-sz)(1-1/sz)(1-z)^2(1+z^L)^2$
15	$2+s+1/s$	$1+2s+2/s$	$-4-2s-2/s$	$-4-s-1/s$	1	$(1-sz)(1-1/sz)(1-z)^2(1-z^L)^2$
16	$-2+s+1/s$	$1-2s-2/s$	0	$-s-1/s$	1	$(1-sz)(1-1/sz)(1+z)^2(1-z^L)^2$

Then the energies of the fermionic excitations are given by $\Lambda = 0$ (twice) and, using equation (3.9), by

$$\Lambda_n = \frac{1}{2}\sin\left(\frac{n\pi}{2L+1}\right) \qquad n = 1, \ldots, L. \tag{6.2}$$

The energies of the fermionic excitations in the other cases from table 1 have a similar form. However, in the cases 10, 11 and 13–16 there is always one solution with roots $z = s^{\pm 1}$ leading to a fermionic energy $\Lambda = \frac{1}{4}(\sqrt{s} + \sqrt{1/s})$ which is—in contrast to the fermionic energies obtained in equation (6.2)—independent of the lattice length L. We will see later [23] that this energy can be connected to a boundary bound state. The nature of this state will be elucidated by studying the corresponding spatial profiles and by comparing some spatial profiles for special choices of the parameters to a Bethe ansatz solution of the XX-chain with only diagonal boundary terms [19]. This will be described in detail in [23].

We now consider case 9 of table 1 which is special because the roots of the polynomial all depend on a parameter s and in general do not lie on the unit circle. Therefore, we will briefly present the corresponding results here. For L even we obtain the solutions $\Lambda = 0$ and

$$\begin{aligned}
\Lambda_n &= \frac{1}{2}\sin\left(\frac{(2n+1)\pi}{2(L+1)} + \frac{\mathrm{i}\ln s}{2(L+1)}\right) \qquad n = 0, 1, \ldots, \frac{L}{2} \\
\Lambda_n &= \frac{1}{2}\sin\left(\frac{(2n+1)\pi}{2(L+1)} - \frac{\mathrm{i}\ln s}{2(L+1)}\right) \qquad n = 0, 1, \ldots, \frac{L-2}{2}
\end{aligned} \tag{6.3}$$

for $|\mathrm{Im}(\ln s)| \leqslant \pi$.

For L odd we have accordingly $\Lambda = 0$, and

$$\begin{aligned}
\Lambda_n &= \frac{1}{2}\sin\left(\frac{n\pi}{L+1} + \frac{\mathrm{i}\ln s}{2(L+1)}\right) \qquad n = 1, \ldots, \frac{L+1}{2} \\
\Lambda_n &= \frac{1}{2}\sin\left(\frac{n\pi}{L+1} - \frac{\mathrm{i}\ln s}{2(L+1)}\right) \qquad n = 0, 1, \ldots, \frac{L-1}{2}
\end{aligned} \tag{6.4}$$

for $0 \leqslant \mathrm{Im}(\ln s) \leqslant \pi$. For $-\pi \leqslant \mathrm{Im}(\ln s) \leqslant 0$ one has to interchange the limits of n in the two sets of eigenvalues given by equation (6.4).

In this example, we can see explicitly how the parameter s appears in the spectrum. The argument of the sine is shifted by the s-dependent term $\mathrm{i}\ln s/(2L+2)$.

For the examples given in table 1, it is also possible to calculate the ground-state energies exactly. The corresponding expressions will be given in the next section.

7. Exact expressions for the ground-state energies of H_{long}

Let us first consider case 4 of table 1 again. The ground-state energy is given by summing up all negative eigenvalues of M (cf (2.16)) and this leads to

$$E_0 = -\frac{1}{2}\sum_{n=1}^{L}\sin\left(\frac{n\pi}{2L+1}\right) = -\frac{1}{4}\cot\frac{\pi}{4L+2}. \tag{7.1}$$

In case 9, also discussed in section 6, the ground-state energy for L even is given by

$$\begin{aligned}
E_0 = -\frac{1}{2}\sum_{n=0}^{(L-2)/2}&\left[\sin\left(\frac{(2n+1)\pi}{2(L+1)} + \frac{\mathrm{i}\ln s}{2(L+1)}\right) + \sin\left(\frac{(2n+1)\pi}{2(L+1)} - \frac{\mathrm{i}\ln s}{2(L+1)}\right)\right] \\
&-\frac{1}{2}\cosh\left(\frac{\ln s}{2L+2}\right) = -\frac{1}{2}\frac{\cosh\left(\ln(s)/(2L+2)\right)}{\sin(\pi/(2L+2))}.
\end{aligned} \tag{7.2}$$

For L odd we obtain

$$E_0 = -\frac{1}{2}\left[\cot\frac{\pi}{2L+2}\cosh\frac{\ln(s)}{2L+2} + \mathrm{i}\sinh\frac{\ln(s)}{2L+2}\right]$$
$$= -\frac{1}{2}\frac{\cosh((\ln(s)+\mathrm{i}\pi)/(2L+2))}{\sin(\pi/(2L+2))}. \tag{7.3}$$

This expression is indeed real if the original Hamiltonian is chosen to be Hermitian. This can be seen by imposing Hermitian boundary terms in the Hamiltonian $\alpha_- = \alpha_+^*$, $\beta_+ = \beta_-^*$ and solving the system of equations

$$A = 2 = 2(-1 + |\alpha_-|^2 + |\beta_+|^2)$$
$$B = 1 = (1 - 2|\alpha_-|^2)(1 - 2|\beta_+|^2)$$
$$(-1)^L C = s + (1/s) = (-1)^L 2|\alpha_-|^2|\beta_+|^2\cos 2(\xi_\alpha + \xi_\beta) \tag{7.4}$$

where ξ_α and ξ_β are the phases of α_- and β_+, respectively. These equations have only the solution $|\alpha_-| = |\beta_+| = 1$, $s = (-1)^L \exp\left(\pm 2\mathrm{i}(\xi_\alpha + \xi_\beta)\right)$. For this choice of s the ground-state energies given by equations (7.2) and (7.3) are always real.

In table 2, the expressions for the ground-state energies for all cases from table 1 are listed. Again, they correspond to H_{long}. In section 12, we will describe how the corresponding ground-state energies for the original Hamiltonian H are obtained from the ones for H_{long}. It is remarkable that despite the non-diagonal boundary terms all expressions for the ground-state energies of H_{long} are given in terms of trigonometric functions. The only exception is case 10 where hyperbolic functions appear in the expression for the ground-state energy (see (7.2) and (7.3)). However, even in this case the model is integrable.

The virtue of table 2 is that one can explicitly see how the ground-state energy is changing with different boundary parameters (we refer to table 3 of section 12 for some examples in which boundary parameters of the Hamiltonian correspond to a given choice of the A, B, C, D and E). This is especially interesting when studying the thermodynamic limit as we will do in [24]. There we will show that the Hamiltonian with arbitrary boundary terms corresponds to a conformal invariant theory. In particular, if one expands the expressions of table 2 in powers of $1/L$, one can already see that they have the typical form of the ground-state expansion corresponding to a conformally invariant theory and one can directly read off the conformal charge and the surface free energy for the different boundary parameters.

Notice that the table includes a well known spin chain: the XX-chain with open boundaries is case 10 with $s = -1$.

The s-dependent cases 9–16 are of special interest because the s-dependence is still manifest in the expressions of the ground-state energy and one can see how this family of ground states varies with s. Note that in all cases 10–16 the s-dependent terms appear additively to the L-dependent part of the ground-state energy (and therewith contribute additively to the surface free energy in the expansion for $L \to \infty$). The physical consequences of the L-independent solutions will be discussed in the next paper in connection with boundary states [23].

In case 9, however, there is no such simple structure and the parameter s is coupled with L as argument of the cosh term. Indeed, case 9 is special as can be seen already from table 1 (the s-dependence appears in the factors of the polynomial which have degree $L + 1$, and not in the factors of degree 1 or 2 as in all other s-dependent cases). This case will be discussed in detail in the following two articles [23, 24].

8. Example of a spectrum of H_{long} with asymmetric bulk terms

Up to now, we have not looked explicitly at Hamiltonians with asymmetric bulk terms, which we mentioned in the introduction. Recall that we can map such a Hamiltonian $\tilde{H}$ given by

Table 2. Ground state energy of H_{long} for the cases from table 1.

Case	L even and L odd	
1	$\frac{1}{4}-\frac{1}{4}\left(\sin\frac{\pi}{4L+6}\right)^{-1}$	
2	$\frac{1}{4}-\frac{1}{4}\left(\left(\sin\frac{\pi}{2L+2}\right)^{-1}+\cot\frac{\pi}{2L+2}\right)$	
4	$-\frac{1}{4}\cot\frac{\pi}{4L+2}$	
11	$\frac{1}{4}-\frac{1}{4}\left(\sin\frac{\pi}{4L+2}\right)^{-1}-\frac{1}{4}(s^{1/2}+s^{-1/2})$	
	L even	L odd
3	$\frac{1}{2}-\frac{1}{4}\left(\left(\sin\frac{\pi}{2L+2}\right)^{-1}+\cot\frac{\pi}{2L+4}\right)$	$\frac{1}{2}-\frac{1}{4}\left(\left(\sin\frac{\pi}{2L+4}\right)^{-1}+\cot\frac{\pi}{2L+2}\right)$
5	$\frac{1}{2}-\frac{1}{4}\left(\left(\sin\frac{\pi}{2L+6}\right)^{-1}+\left(\sin\frac{\pi}{2L+2}\right)^{-1}\right)$	$\frac{1}{2}-\frac{1}{4}\left(\cot\frac{\pi}{2L+2}+\cot\frac{\pi}{2L+6}\right)$
6	$\frac{1}{2}-\frac{1}{2}\cot\frac{\pi}{2L+4}$	$\frac{1}{2}-\frac{1}{2}\left(\sin\frac{\pi}{2L+4}\right)^{-1}$
7	$\frac{1}{4}-\frac{1}{4}\left(\left(\sin\frac{\pi}{2L+2}\right)^{-1}+\left(\sin\frac{\pi}{2L+4}\right)^{-1}\right)$	$\frac{1}{4}-\frac{1}{4}\left(\cot\frac{\pi}{2L+2}+\cot\frac{\pi}{2L+4}\right)$
8	$\frac{1}{4}-\frac{1}{4}\left(\cot\frac{\pi}{2L+2}+\cot\frac{\pi}{2L+4}\right)$	$\frac{1}{4}-\frac{1}{4}\left(\left(\sin\frac{\pi}{2L+2}\right)^{-1}+\left(\sin\frac{\pi}{2L+4}\right)^{-1}\right)$
9	$-\frac{1}{2}\left(\cosh\frac{\ln(s)}{2L+2}\right)\left(\sin\frac{\pi}{2L+2}\right)^{-1}$	$-\frac{1}{2}\left(\cosh\frac{\ln(s)+\mathrm{i}\pi}{2L+2}\right)\left(\sin\frac{\pi}{2L+2}\right)^{-1}$
10	$\frac{1}{2}-\frac{1}{2}\left(\sin\frac{\pi}{2L+2}\right)^{-1}-\frac{1}{4}(s^{1/2}+s^{-1/2})$	$\frac{1}{2}-\frac{1}{2}\cot\frac{\pi}{2L+2}-\frac{1}{4}(s^{1/2}+s^{-1/2})$
12	$\frac{1}{2}-\frac{1}{2}\cot\frac{\pi}{2L}-\frac{1}{4}(s^{1/4}+s^{-1/4})$ $-\frac{\mathrm{i}}{4}(s^{1/4}-s^{-1/4})$	$\frac{1}{2}-\frac{1}{2}\left(\sin\frac{\pi}{2L}\right)^{-1}-\frac{1}{4}(s^{1/4}+s^{-1/4})$ $-\frac{\mathrm{i}}{4}(s^{1/4}-s^{-1/4})$
13	$\frac{1}{2}-\frac{1}{2\sqrt{2}}-\frac{1}{2}\cot\frac{\pi}{2L}-\frac{1}{4}(s^{1/2}+s^{-1/2})$	$\frac{1}{2}-\frac{1}{2\sqrt{2}}-\frac{1}{2}\left(\sin\frac{\pi}{2L}\right)^{-1}-\frac{1}{4}(s^{1/2}+s^{-1/2})$
14	$-\frac{1}{2}\left(\sin\frac{\pi}{2L}\right)^{-1}-\frac{1}{4}(s^{1/2}+s^{-1/2})$	$-\frac{1}{2}\cot\frac{\pi}{2L}-\frac{1}{4}(s^{1/2}+s^{-1/2})$
15	$-\frac{1}{2}\cot\frac{\pi}{2L}-\frac{1}{4}(s^{1/2}+s^{-1/2})$	$-\frac{1}{2}\left(\sin\frac{\pi}{2L}\right)^{-1}-\frac{1}{4}(s^{1/2}+s^{-1/2})$
16	$\frac{1}{2}-\frac{1}{2}\cot\frac{\pi}{2L}-\frac{1}{4}(s^{1/2}+s^{-1/2})$	$\frac{1}{2}-\frac{1}{2}\left(\sin\frac{\pi}{2L}\right)^{-1}-\frac{1}{4}(s^{1/2}+s^{-1/2})$

equation (1.2) to a Hamiltonian H of the form given by (1.1) which has symmetric bulk terms and L-dependent boundary terms of the special form given by (1.3). Using the methods previously described, we can solve the eigenvalue problem for the Hamiltonian H_{long} and in this way obtain the spectrum of $\tilde{H}_{\text{long}}$, where $\tilde{H}_{\text{long}}$ is obtained from $\tilde{H}$ in the same way as H_{long} from H by adding one site at each end of the chain. We will carry this out for one example.

We choose a Hamiltonian $\tilde{H}_{\text{long}}$ whose transformed H_{long} has boundary terms corresponding to case 9. Notice that this is the only factorizable case where this can be done independently of L if $p \neq q$, i.e. the analysis can simultanously be carried out for all Hamiltonians $\tilde{H}$ of the chosen type with arbitrary length. In all other cases, starting from one factorizable case and changing the length L would result in boundary parameters belonging to another (perhaps not even factorizable) case.

One possible choice for the boundary parameters in case 9 is given by (as can be directly seen from (4.2))

$$\alpha_-\alpha_+ = 1 \qquad \beta_+\beta_- = 1 \qquad (-1)^L(\alpha_-^2\beta_+^2 + \alpha_+^2\beta_-^2) = s + \frac{1}{s} \qquad \alpha_z = 0 = \beta_z.$$

Expressing α_- in terms of α_+ and β_- in terms of β_+ and using equation (1.3), we obtain

$$s = (-1)^L\left(\frac{\beta'_+}{\alpha'_+}\right)^2 Q^{2-2L} \qquad \left(\text{or } 1/s = (-1)^L\left(\frac{\beta'_+}{\alpha'_+}\right)^2 Q^{2-2L}\right).$$

Using the results obtained in equation (6.3) we get for the fermionic excitations for even L

$$\Lambda = \frac{1}{2}\sin\left(\frac{(2n+1)\pi}{2L+2} \pm \mathrm{i}\left[\frac{(2\ln Q + \ln(\beta'_+/\alpha'_+))}{L+1} - \ln Q\right]\right) \qquad n = 0, \ldots, \frac{L-2}{2}$$

$$\Lambda = \frac{1}{2}\cosh\left[\frac{2\ln Q + \ln(\beta'_+/\alpha'_+)}{L+1} - \ln Q\right]. \tag{8.1}$$

The quasi-momenta $(2n+1)\pi/(2L+2)$ are shifted by the constant

$$\mathrm{i}\left[\frac{2\ln Q + \ln(\beta'_+/\alpha'_+)}{L+1} - \ln Q\right].$$

The second L-independent term of this constant is typical for asymmetric bulk terms as will be seen in [24]. A similar expression has been obtained in [8] for the fermionic excitations of $\tilde{H}$ with totally asymmetric bulk terms ($p = 1, q = 0$), $\alpha_- \neq 0$, $\beta_+ \neq 0$ and $\alpha_+ = \beta_- = \alpha_z = \beta_z = 0$.

The ground-state energy is given by summing up all negative eigenvalues of M, leading to

$$E_0 = -\cosh\left(\frac{\ln(q\beta'_+/p\alpha'_+)}{L+1} - \ln Q\right)\left(2\sin\left(\frac{\pi}{2L+2}\right)\right)^{-1}. \tag{8.2}$$

Observe that for $p/q = 1$ we obtain the previous expression calculated for case 9.

9. Projection method and the σ^x one-point functions

Up to now we have dealt only with the Hamiltonian H_{long} given by equation (2.1) which was obtained from H (see (1.2)) by adding one lattice site at each end of the chain. In this section we will explain how the spectrum of H is related to the spectrum of H_{long}.

Since, as mentioned in section 2, σ_0^x and σ_{L+1}^x commute with H_{long} the spectrum decomposes into four sectors $(++, +-, -+, --)$ corresponding to the eigenvalues ± 1 of σ_0^x and σ_{L+1}^x. The eigenvalues and eigenvectors of H are related to the $(++)$-sector in the following way.

If $|E\rangle$ is an eigenvector of H corresponding to an eigenvalue E then $|E_{\text{long}}\rangle = |+\rangle \otimes |E\rangle \otimes |+\rangle$ is an eigenvector of H_{long} corresponding to the same eigenvalue E, where $\sigma_0^x|+\rangle = |+\rangle$ and $|E_{\text{long}}\rangle$ is an element of the space $\mathbb{C}^2 \otimes \mathbb{C}^L \otimes \mathbb{C}^2$. Thus the whole spectrum of H is contained in the spectrum of H_{long} projected onto the $(++)$-sector. Since the dimension of the $(++)$-sector is 2^L, we conclude that the spectrum of H is identical to the spectrum of H_{long} projected onto the $(++)$-sector.

Before describing how we will proceed to project to the (++)-sector, we make some definitions which are needed later. First, we want to remind the reader that M defined by equation (2.11) always has a twofold degenerate eigenvalue 0 corresponding to the eigenvectors $(0, 1, 0, 0, \ldots)$ and $(0, 0, \ldots, 1, 0)$ of M. Using the Clifford operators $\tau_j^{\pm}$ given by equation (2.3), we now define the corresponding ladder operators

$$b_0 = (\tau_0^+ - \mathrm{i}\tau_{L+1}^-)/2 \qquad a_0 = (\tau_0^+ + \mathrm{i}\tau_{L+1}^-)/2. \tag{9.1}$$

We also define the vacuum representation with the lowest weight vector $|\mathrm{vac}\rangle$ by

$$a_k|\mathrm{vac}\rangle = 0 \qquad \forall k. \tag{9.2}$$

Because we are interested in eigenstates of σ_0^x and σ_{L+1}^x we define the vectors

$$|v^{\pm}\rangle = \tfrac{1}{\sqrt{2}}(|\mathrm{vac}\rangle \pm |0\rangle) \tag{9.3}$$

where $|0\rangle = b_0|\mathrm{vac}\rangle$. Observe that

$$\sigma_0^x|v^{\pm}\rangle = \pm|v^{\pm}\rangle. \tag{9.4}$$

Now we will proceed in three steps. In the first step (subsection 9.1) we will show, using some algebraic considerations, that the vectors $|v^{\pm}\rangle$ are also eigenvectors of σ_{L+1}^x. It will turn out that the eigenvalues of σ_{L+1}^x corresponding to the eigenvectors $|v^+\rangle$ and $|v^-\rangle$ always have opposite signs, i.e.

$$\sigma_{L+1}^x|v^{\pm}\rangle = \pm\eta|v^{\pm}\rangle \tag{9.5}$$

with $\eta^2 = 1$. The value of η plays a crucial role in the following. We will also show that the (++)-sector consists either of the states

$$\prod_{j=1}^{r} b_{k_j}|v^+\rangle \qquad \text{with } r \text{ even} \tag{9.6}$$

or

$$\prod_{j=1}^{r} b_{k_j}|v^-\rangle \qquad \text{with } r \text{ odd} \tag{9.7}$$

where $0 < k_j \leqslant k_{j+1}$. Since $k_j \neq 0$, the creation operator of the spurious zero mode defined by equation (9.1) does not appear in (9.6) and (9.7). The ground state of H corresponds to $|v^+\rangle$ or to $b_{\mathrm{lowest}}|v^-\rangle$, where b_{lowest} denotes the creation operator corresponding to the fermionic energy with smallest real part and $k \neq 0$.

Whether the (++)-sector consists of the states (9.6) or (9.7) will be shown to depend on the value of η (see (9.5)) which will be calculated by computing the expectation value $\langle v^+|\sigma_{L+1}^x|v^+\rangle$. Note that we define $\langle v^{\pm}|$ via

$$\langle v^{\pm}| = \tfrac{1}{\sqrt{2}}(\langle\mathrm{vac}| \pm \langle\mathrm{vac}|a_0) \tag{9.8}$$

where $\langle\mathrm{vac}|$ denotes the left vacuum of H_{long}, i.e.

$$\langle\mathrm{vac}|b_k = 0. \tag{9.9}$$

Note that if H_{long} is not Hermitian, $\langle\mathrm{vac}|$ is not equal to $|\mathrm{vac}\rangle^{\dagger}$ in general.

In the second step (section 10), we will show how to calculate the one-point function

$$f(j) = \langle v^+|\sigma_j^x|v^+\rangle. \tag{9.10}$$

In the present context, this is done merely for technical reasons in order to calculate $f(L+1)$; however, it will be essential in another context. Namely, the explicit calculation of $f(j)$ will

be presented in the following paper [23]. We would already like to remark that the calculation of $f(j)$ is similar to the calculation of the two-point function

$$g(i, j) = \langle v^+|\sigma_i^x \sigma_j^x|v^+\rangle. \tag{9.11}$$

Note that, due to equation (9.4), one already sees that $f(j) = g(0, j)$. We show in section 10 that the functions $f(j)$ and $g(i, j)$ are both given by Pfaffians of submatrices of the same matrix. We will, furthermore, generalize these considerations to states of the form (9.6) and (9.7). These results also apply to H although we started with the larger space of states of H_{long}.

Using equations (2.40) and (2.42), we will obtain determinant representations for $f(j)$ and $g(i, j)$ which can be treated analytically in the calculation of $f(L + 1)$. This calculation can be found in section 11 and will be the third step.

9.1. Algebraic considerations

In this subsection, we will show that the (++)-sector consists either of the states given by (9.6) or (9.7) and clarify the role of η given in (9.5). Because

$$(\phi_k^{\pm})_0^+ = (\phi_k^{\pm})_{L+1}^- = 0 \qquad \forall k \neq 0 \tag{9.12}$$

which can be seen directly from the matrix M, we obtain the commutation relations

$$[\sigma_{L+1}^x, b_k] = [\sigma_{L+1}^x, a_k] = \{\sigma_0^x, b_k\} = \{\sigma_0^x, a_k\} = 0 \qquad \forall k \neq 0 \tag{9.13}$$

from equations (2.18) and (2.17) and therefore

$$[\sigma_0^x, N_k] = [\sigma_{L+1}^x, N_k] = 0 \qquad \forall k \neq 0. \tag{9.14}$$

Due to equation (9.14) the vectors $|v^{\pm}\rangle$ have to be eigenvectors of σ_{L+1}^x, i.e.

$$\sigma_{L+1}^x|v^{\pm}\rangle = \eta^{\pm}|v^{\pm}\rangle. \tag{9.15}$$

Thus the sector containing $|v^+\rangle$ respectively $|v^-\rangle$ is well defined and given by the values of η^+ and η^-, respectively. Note that (9.15) is not as precise as (9.5) because (9.5) implies $\eta^+ = -\eta^-$.

Due to equations (9.13) we can make the following statement concerning the vectors of a given sector. If an arbitrary vector $|v\rangle$ is an element of the $(\pm\epsilon)$-sector where $\epsilon \in \{+, -\}$, then $b_k|v\rangle$ with $k \neq 0$ is an element of the $(\mp\epsilon)$-sector. Now one has to distinguish two cases.

(i) If $|v^+\rangle$ is an element of the (++)-sector, i.e. $\eta^+ = +1$, then all the states given by (9.6) are also elements of the (++)-sector. The vector $|v^-\rangle$ then has to be an element of the $(--)$-sector because otherwise the $(--)$-sector would be missing in the space of states, which is not the case. Thus, we have $\eta^- = -1$.

(ii) If $|v^+\rangle$ is an element of the $(+-)$-sector, i.e. $\eta^+ = -1$, then $|v^-\rangle$ has to be an element of the $(-+)$-sector. Otherwise $|v^-\rangle$ would be an element of the $(--)$-sector and there would be no (++)-sector. As a consequence, we have that $\eta^- = +1$ and all the states given by (9.7) are elements of the (++)-sector.

In both cases, the subspace spanned by the vectors (9.6) respectively (9.7) has dimension 2^L and thus they form a basis of the (++)-sector. Because the values of η^+ and η^- always have opposite signs, we will use the variable η defined by equation (9.5) in the following.

10. One- and two-point functions of σ^x

In this section we show how to compute the one- and two-point functions for the σ_j^x operator with respect to the states $|v^{\pm}\rangle$ defined by equation (9.3) and $\langle v^{\pm}|$ defined by (9.8) following

the method of Lieb, Schultz and Mattis (LSM) [1]. The computation of the correlators of the operators σ_j^y can be done similarly. In this paper, however, we are only interested in the value of $\langle v^+|\sigma_j^x|v^+\rangle$ at the particular point $j = L+1$ which is calculated in section 11 using the results of this section. Due to equation (9.5) we thereby obtain the value of η which is needed for the projection from H_{long} to H as described in the previous section. The calculation for general values of j will be part of the second paper of this series [23].

The main difference in comparison to the problem of LSM [1] is that in our case the one-point functions do not vanish because of the non-diagonal boundary terms we are considering. They can be calculated in the same way as the two-point correlators. At the end of this section, we will briefly note how to compute the one- and two-point functions for excited states of H_{long} of the form (9.6) and (9.7). This is not necessary for the calculation of η defined in equation (9.5), but it is needed for the calculation of the one- and two-point functions for the eigenstates of H. Note that if $\eta = -1$ the ground state of H corresponds to an excited state of H_{long}.

We now proceed to the calculation of the one- and two-point functions. Writing σ_j^x in terms of the $\tau_i^\pm$ defined in equation (2.3), we obtain

$$\langle v^\pm|\sigma_j^x|v^\pm\rangle = \pm(-\mathrm{i})^j\langle v^\pm|\tau_0^-\prod_{k<j}\tau_k^+\tau_k^-\tau_j^+|v^\pm\rangle \tag{10.1}$$

which is up to the sign exactly the two-point function $\langle v^\pm|\sigma_0^x\sigma_j^x|v^\pm\rangle$. In general,

$$\langle v^\pm|\sigma_i^x\sigma_j^x|v^\pm\rangle = (-\mathrm{i})^{j-i}\langle v^\pm|\tau_i^-\prod_{k<j}\tau_k^+\tau_k^-\tau_j^+|v^\pm\rangle. \tag{10.2}$$

Of course, i denotes $\sqrt{-1}$. Using equation (2.24), $\tau_j^\pm$ can be expressed in terms of ladder operators a_k and b_k, i.e.

$$\tau_j^\mu = \sum_{k=0}^{L+1}(\phi_k^-)_j^\mu a_k + (\phi_k^+)_j^\mu b_k. \tag{10.3}$$

Because $(\phi_0^\pm)_j^\mu$ is only different from zero if either $j = 0$ and $\mu = +$ or $j = L+1$ and $\mu = -$ (compare equations (9.1) and (2.18) and (2.17)) we have

$$\langle v^\pm|\tau_i^-\prod_{k<j}\tau_k^+\tau_k^-\tau_j^+|v^\pm\rangle = \langle\mathrm{vac}|\tau_i^-\prod_{k<j}\tau_k^+\tau_k^-\tau_j^+|\mathrm{vac}\rangle. \tag{10.4}$$

For simplicity, we will denote $\langle\mathrm{vac}|\hat{O}|\mathrm{vac}\rangle$ by $\langle\hat{O}\rangle$ in the following where $\hat{O}$ denotes an arbitrary operator. Using Wick's theorem we are left with the calculation of the Pfaffian of the antisymmetric matrix $\mathbf{A}$, i.e.

$$\left\langle\tau_i^-\prod_{k<j}\tau_k^+\tau_k^-\tau_j^+\right\rangle = \mathrm{Pf}\,\mathbf{A} \tag{10.5}$$

where

$$\mathbf{A} = \begin{pmatrix} 0 & \langle\tau_i^-\tau_{i+1}^+\rangle & \langle\tau_i^-\tau_{i+1}^-\rangle & \langle\tau_i^-\tau_{i+2}^+\rangle & \cdots & \langle\tau_i^-\tau_j^+\rangle \\ \langle\tau_{i+1}^+\tau_i^-\rangle & 0 & \langle\tau_{i+1}^+\tau_{i+1}^-\rangle & \langle\tau_{i+1}^+\tau_{i+2}^+\rangle & \cdots & \langle\tau_{i+1}^+\tau_j^+\rangle \\ \langle\tau_{i+1}^-\tau_i^-\rangle & \langle\tau_{i+1}^-\tau_{i+1}^+\rangle & 0 & \langle\tau_{i+1}^-\tau_{i+2}^+\rangle & \cdots & \langle\tau_{i+1}^-\tau_j^+\rangle \\ \langle\tau_{i+2}^+\tau_i^-\rangle & \langle\tau_{i+2}^+\tau_{i+1}^+\rangle & \langle\tau_{i+2}^+\tau_{i+1}^-\rangle & 0 & \cdots & \langle\tau_{i+2}^+\tau_j^+\rangle \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \langle\tau_j^+\tau_i^-\rangle & \langle\tau_j^+\tau_{i+1}^+\rangle & \langle\tau_j^+\tau_{i+1}^-\rangle & \langle\tau_j^+\tau_{i+2}^+\rangle & \cdots & 0 \end{pmatrix}. \tag{10.6}$$

We want to remind the reader that the Pfaffian of a $2n \times 2n$ antisymmetric matrix A with matrix elements a_{ij} is defined by

$$\mathrm{Pf}A = \frac{1}{n!2^n} \sum_{\sigma \in S_{2n}} \mathrm{sgn}(\sigma) a_{\sigma(1)\sigma(2)} a_{\sigma(3)\sigma(4)} \dots a_{\sigma(2n-1)\sigma(2n)} \tag{10.7}$$

where S_{2n} denotes the symmetric group of degree $2n$.

The expectation values of the basic contractions of pairs which form the entries of $\mathbf{A}$ are evaluated using equation (10.3). Due to the property of $\langle \mathrm{vac}|$ (cf (9.9)) we obtain

$$\langle \tau_i^\mu \tau_j^\nu \rangle = \sum_{k=0}^{L+1} (\phi_k^-)_i^\mu (\phi_k^+)_j^\nu. \tag{10.8}$$

In general, no further simplification is possible.

Nevertheless, there exist two special cases where the calculation of the Pfaffian can be reduced to the calculation of a determinant. Namely, this is possible if no diagonal boundary terms are present or if $\alpha_- = \alpha_+$ and $\beta_- = \beta_+$. This reduction uses the additional relations for the eigenvectors given by equations (2.40) or (2.42), respectively. Note that in this paper the general relation $(\mathrm{Pf}\,\mathbf{A})^2 = \det \mathbf{A}$ is of no use because we are exactly interested in the sign of η.

In the absence of diagonal boundaries we can use equation (2.40) to simplify (10.8). Using similar arguments as LSM we also obtain a determinant representation for the correlation functions; however, the contributing contractions are different from theirs. In fact, using equation (2.40) results in

$$\langle \tau_i^\mu \tau_j^\nu \rangle = 0 \qquad \text{for } i + j \text{ even} \tag{10.9}$$

and thus the correlation functions are given by subdeterminants of the $(L+1) \times (L+1)$ matrix

$$\mathbf{D} = \begin{pmatrix} \langle \tau_0^- \tau_1^+ \rangle & \langle \tau_0^- \tau_1^- \rangle & \langle \tau_0^- \tau_3^+ \rangle & \cdots \\ \langle \tau_2^+ \tau_1^+ \rangle & \langle \tau_2^+ \tau_1^- \rangle & \langle \tau_2^+ \tau_3^+ \rangle & \cdots \\ \langle \tau_2^- \tau_1^+ \rangle & \langle \tau_2^- \tau_1^- \rangle & \langle \tau_2^- \tau_3^+ \rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{10.10}$$

Denoting by $\mathbf{D}_j^i$ the matrix $\mathbf{D}$ after elimination of the first i rows and columns and the last $L+1-j$ rows and columns we can write

$$\mathrm{Pf}\,\mathbf{A} = \mathrm{i}^{j-i} f_{ij} \det \mathbf{D}_j^i \tag{10.11}$$

where

$$f_{ij} = \begin{cases} -\mathrm{i} & \text{if } i \text{ even and } j \text{ odd} \\ \mathrm{i} & \text{if } i \text{ odd and } j \text{ even} \\ 1 & \text{otherwise.} \end{cases} \tag{10.12}$$

The calculation of $\mathrm{Pf}\,\mathbf{A}$ also simplifies if $\alpha_+ = \alpha_-$ and $\beta_+ = \beta_-$. In this case we can utilize equation (2.42) to obtain

$$\langle \tau_i^\mu \tau_j^\mu \rangle = 0. \tag{10.13}$$

This again results in a determinant representation of $\mathrm{Pf}\,\mathbf{A}$, i.e.

$$\mathrm{Pf}\,\mathbf{A} = \begin{vmatrix} \langle \tau_i^- \tau_{i+1}^+ \rangle & \langle \tau_i^- \tau_{i+2}^+ \rangle & \cdots & \langle \tau_i^- \tau_j^+ \rangle \\ \langle \tau_{i+1}^- \tau_{i+1}^+ \rangle & \langle \tau_{i+1}^- \tau_{i+2}^+ \rangle & \cdots & \langle \tau_{i+1}^- \tau_j^+ \rangle \\ \vdots & \vdots & & \vdots \\ \langle \tau_{j-1}^- \tau_{i+1}^+ \rangle & \langle \tau_{j-1}^- \tau_{i+2}^+ \rangle & \cdots & \langle \tau_{j-1}^- \tau_j^+ \rangle \end{vmatrix}. \tag{10.14}$$

By simple modifications one can generalize the results of this section to excited states of the form (9.6) or (9.7). The argument runs as follows. Any state given by elementary excitations can be regarded as the vacuum state $|\mathrm{vac}'\rangle$ of a new set of ladder operators, where the a_k and b_k of the excited fermions are interchanged. This corresponds to an interchange of the eigenvectors ϕ_k^- and ϕ_k^+ (see (2.17) and (2.18)). Thus the calculation of correlation functions for the states in (9.6) and (9.7) is equivalent to the calculation of the correlation functions for the states $|v^{+\prime}\rangle$ defined in the same way as $|v^+\rangle$ in equation (9.3) but now using

$$|\mathrm{vac}'\rangle = \prod_{j=1}^{r} b_{k_j}|\mathrm{vac}\rangle \tag{10.15}$$

as vacuum state where r is even or odd, respectively, and $k \neq 0$. The left vacuum defined by equation (9.9) has to be modified analogously. As a consequence, we only have to replace equation (10.8) by

$$\langle \tau_i^\mu \tau_j^\nu \rangle = \sum_{k\ \mathrm{unexc.}} (\phi_k^-)_i^\mu (\phi_k^+)_j^\nu + \sum_{k\ \mathrm{exc.}} (\phi_k^+)_i^\mu (\phi_k^-)_j^\nu. \tag{10.16}$$

11. Calculation of $\langle \sigma_{L+1}^x \rangle$

If the diagonal boundary terms are absent or if $\alpha_+ = \alpha_-$ and $\beta_+ = \beta_-$, we can make use of equations (10.11) or (10.14), respectively, in order to calculate

$$\eta = \langle v^+ | \sigma_{L+1}^x | v^+ \rangle. \tag{11.1}$$

Recall that we need the value of η to decide whether the $(++)$-sector of the space of states of H_{long} is given by the states of the form (9.6) or (9.7).

Thus, if no diagonal boundary terms are present, we have to calculate $\det \mathbf{D}$, where $\mathbf{D}$ is defined by equation (10.10). This determinant can be written as the product of two determinants

$$(-1)^L \det \mathbf{D} = \det \mathbf{A}_g \det \mathbf{A}_u \tag{11.2}$$

where

$$\mathbf{A}_g = \begin{pmatrix} (\phi_1^-)_0^- & (\phi_2^-)_0^- & (\phi_3^-)_0^- & \cdots \\ (\phi_1^-)_2^- & (\phi_2^-)_2^- & (\phi_3^-)_2^- & \cdots \\ (\phi_1^-)_2^+ & (\phi_2^-)_2^+ & (\phi_3^-)_2^+ & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\mathbf{A}_u = \begin{pmatrix} (\phi_1^+)_1^- & (\phi_1^+)_1^+ & (\phi_1^+)_3^- & \cdots \\ (\phi_2^+)_1^- & (\phi_2^+)_1^+ & (\phi_2^+)_3^- & \cdots \\ (\phi_3^+)_1^- & (\phi_3^+)_1^+ & (\phi_3^+)_3^- & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{11.3}$$

The factor $(-1)^L$ is due to permutations of rows and columns which can be seen by comparing the product $\mathbf{A}_g\mathbf{A}_u$ with $\mathbf{D}$. Without loss of generality, we may assume that the eigenvectors are normalized in such a way that they satisfy equation (2.38) with $c = 1$. Using equation (2.40) we then find

$$\mathbf{A}_g \mathbf{A}_g^{\mathrm{t}} = \mathbf{1} \qquad \mathbf{A}_u \mathbf{A}_u^{\mathrm{t}} = -\mathbf{1}. \tag{11.4}$$

Due to the special form of the matrix M (see equation (2.32)) and (2.38), the two matrices $\mathbf{A}_g$ and $\mathbf{A}_u$ are related by a matrix $\mathbf{M}_{g\to u}$ via

$$\mathbf{\Lambda}^{-1}\mathbf{M}_{g\to u}\mathbf{A}_g = \mathbf{A}_u^{\mathrm{t}} \tag{11.5}$$

where $\mathbf{\Lambda}_{kk'} = \Lambda_k \delta_{kk'}$ with $k > 0$. The matrix $\mathbf{M}_{g\to u}$ is given by

$$\mathbf{M}_{g\to u} = \begin{pmatrix} -G'^{\mathrm{t}} & F & 0 & 0 & 0 \\ 0 & -F^{\mathrm{t}} & \ddots & 0 & 0 \\ 0 & 0 & \ddots & F & 0 \\ 0 & 0 & 0 & -F^{\mathrm{t}} & K' \end{pmatrix} \tag{11.6}$$

for L odd or

$$\mathbf{M}_{g\to u} = \begin{pmatrix} -G'^{\mathrm{t}} & F & 0 & 0 & 0 \\ 0 & -F^{\mathrm{t}} & \ddots & 0 & 0 \\ 0 & 0 & \ddots & F & 0 \\ 0 & 0 & 0 & -F^{\mathrm{t}} & F \\ 0 & 0 & 0 & 0 & -K'^{\mathrm{t}} \end{pmatrix} \tag{11.7}$$

for L even, where we have denoted by G' the matrix G of equation (2.5) with the second row eliminated and by K' the matrix K of (2.5) with the first column eliminated. Note that the eliminated rows and columns contain only entries which are equal to zero.

Using equations (11.5) and (11.4) in (11.2), we obtain

$$\det \mathbf{D} = (-1)^L \det \mathbf{\Lambda}^{-1} \det \mathbf{M}_{g\to u}. \tag{11.8}$$

The value of $\det \mathbf{M}_{g\to u}$ can be computed in an elementary way,

$$\det \mathbf{M}_{g\to u} = \begin{cases} -(\alpha_-\beta_+ + \alpha_+\beta_-)/4^{L+1} & \text{for L odd} \\ -\mathrm{i}(\alpha_-\beta_+ + \alpha_+\beta_-)/4^{L+1} & \text{for L even.} \end{cases} \tag{11.9}$$

Plugging this into equation (10.11), we end up with

$$\mathrm{Pf}\, \mathbf{A} = (-\mathrm{i})^{L+1} \frac{\alpha_-\beta_+ + \alpha_+\beta_-}{4^{L+1} \prod_{k\neq 0} \Lambda_k}. \tag{11.10}$$

If $\alpha_- = \alpha_+$ and $\beta_- = \beta_+$, we obtain the same result by using equation (10.14) and performing a similar calculation. Combining (10.1), (10.4) and (10.5) with (11.10) we are left in both cases with

$$\eta = \langle v^+ | \sigma^x_{L+1} | v^+ \rangle = (-1)^{L+1} \frac{\alpha_-\beta_+ + \alpha_+\beta_-}{4^{L+1} \prod_{k\neq 0} \Lambda_k}. \tag{11.11}$$

Notice that in these cases the expression of η does not depend on α_z and β_z. It is not possible to calculate the product of all eigenvalues in equation (11.11) in general, but the squared product of eigenvalues can be calculated from $\det M'$ where M' denotes the matrix M with the second and the last but one row and column eliminated. In both cases this yields

$$\det \mathbf{\Lambda}^2 = (-1)^{L+1} \det M' = (\alpha_-\beta_+ + \alpha_+\beta_-)^2 / 4^{2L+2}. \tag{11.12}$$

If the Hamiltonian is Hermitian, the product of eigenvalues is simply given by $\prod_{k\neq 0} \Lambda_k = |\alpha_-\beta_+ + \alpha_+\beta_-|/4^{L+1}$. This also holds for Hamiltonians with only real entries because in these cases the product is real and positive. Thus, we can apply equation (11.11) directly. Otherwise, one would have to know all the eigenvalues explicitly.

Note that the value of η can only change by variation of the boundaries if one crosses a point in the parameter space at which an additional mode with $\mathrm{Re}\Lambda_k = 0$ and $k \neq 0$ exists. This is due to the fact that the eigenvalues of H and H_{long} are continuous functions of the boundary parameters. However, at a point satisfying the above condition the value of η is not well defined, because the corresponding ladder operators a_k and b_k are not well defined as already mentioned in section 2.1. Therefore, one can aquire a change of sign in η by passing through such a point.

If H is Hermitian the condition to have a mode with $\mathrm{Re}\Lambda_k = 0$ and $k \neq 0$ is equivalent to the existence of an additional zero mode. The presence of such a zero mode corresponds to the root $z = -1$ in the polynomial given by equation (4.1). This implies the condition $\alpha_-\beta_+ + \alpha_+\beta_- = 0$. Thus if H is Hermitian, i.e. $\alpha_+ = \alpha_-^*, \beta_+ = \beta_-^*$, we have to only distinguish the two regions $\mathrm{Re}(\alpha_-\beta_+) > 0$ and $\mathrm{Re}(\alpha_-\beta_+) < 0$. Thus, we conclude that if H is Hermitian we obtain the following expression for η:

$$\eta = (-1)^{L+1}\mathrm{sign}(\mathrm{Re}\,(\alpha_-\beta_+)). \tag{11.13}$$

The results of this section, namely equations (11.11) and (11.13), allow us to calculate the ground-state energy of H for the exactly solvable cases of table 1. This will be the subject of section 12.

12. Ground-state energies for the Hamiltonian H in the exactly solvable cases

In section 9 we have shown that the ground state of H corresponds either to $|v^+\rangle$ or to $b_{\mathrm{lowest}}|v^-\rangle$ where b_{lowest} is the creation operator corresponding to the fermion energy with the smallest real part, which we will denote by $2\Lambda_{\mathrm{lowest}}$ in the following, and the $|v^\pm\rangle$ are defined in equation (9.3). Which of these two states corresponds to the ground state depends on the eigenvalue η of $|v^+\rangle$ with respect to the operation of σ^x_{L+1}. The eigenvalue η is either +1 or -1. If $\eta = 1$, then the ground state corresponds to $|v^+\rangle$ and the ground-state energy of H is equal to the ground-state energy of H_{long}. If $\eta = -1$, then the ground-state corresponds to $b_{\mathrm{lowest}}|v^-\rangle$ and the ground-state energy of H is given by the sum of the ground-state energy of H_{long} and $2\Lambda_{\mathrm{lowest}}$. For the exactly solvable cases, the ground-state energies for H_{long} are already contained in table 2.

If at least one of the following conditions is satisfied:

(a) H_{long} is Hermitian,

(b) H_{long} has no σ^z boundary terms ($\alpha_z = 0 = \beta_z$),

(c) $\alpha_- = \alpha_+$ and $\beta_+ = \beta_-$,

the value of η can be easily calculated by using the explicit formulae of section 11. In cases (b) and (c), the expression for η is given in equation (11.11) in terms of α_-, β_+, β_- and α_+ and the eigenvalues Λ_k of M. In case (a) where H_{long} is Hermitian, η is given by equation (11.13) in terms of α_- and β_+ alone. In the other cases, one would have to calculate the Pfaffian of the matrix $\mathbf{A}$ given by equation (10.6) using different methods than those we used in sections 10 and 11 to decide which of the states $|v^+\rangle$ or $b_{\mathrm{lowest}}|v^-\rangle$ corresponds to the ground state of H.

To determine the ground-state energy for a given Hamiltonian H of types (a)–(c) one has to calculate the expression for η given by equation (11.11) or (11.13). Analytically, the ground-state energy for H can be calculated with our methods only for the cases given in table 1 where the polynomial factorizes into cyclotomic polynomials and where one knows the whole spectrum of H_{long}. These cases are given in terms of the parameters A, B, C, D and E. In order to put our machinery to work, we need the corresponding parameters α_-, α_+, β_-, β_+, α_z and β_z. Since the transformation from A, B, C, D and E to α_-, α_+, β_-, β_+, α_z and β_z (which is given in (4.2)) is nonlinear and leads from five to six variables, the choice of the parameters α_-, α_+, β_-, β_+, α_z and β_z for a given set A, B, C, D and E is not unique, creating some freedom of choice.

For all the cases listed in table 1, we solved equations (4.2) for α_-, α_+, β_-, β_+, α_z and β_z and allowed only solutions which additionally satisfied one of the conditions (a)–(c) above. These solutions are listed in table 3. The choices of boundary parameters obtained from those given in table 3 by application of an obvious similarity transformation to the Hamiltonian H,

Table 3. Exactly solvable cases from table 1. Details needed for the projection method.

Case	L	α_z	β_z	α_- α_+ β_+ β_-	s	$2\Lambda_{\text{lowest}}$
1	arb.	0	0	$\alpha_-\alpha_+ = 1\ \beta_+\beta_- = \frac{1}{2}\ \alpha_+\beta_- = \pm\frac{(1\pm\mathrm{i})}{2}$		$\sin\frac{\pi}{4L+6}$
2	arb.	0	0	$\alpha_-\alpha_+ = 1\ \beta_+ = \beta_- = 0$		0
	arb.	0	$\pm\frac{1}{\sqrt{2}}$	$\alpha_- = \pm\frac{1}{\sqrt{2}}\mathrm{e}^{\mathrm{i}\phi}\ \alpha_+ = \pm\frac{1}{\sqrt{2}}\mathrm{e}^{-\mathrm{i}\phi}$ $\beta_+ = \beta_- = 0$		0
3	arb.	0	0	$\alpha_-\alpha_+ = \frac{1}{2}\ \beta_+ = \beta_- = 0$		0
4	arb.	0	$\pm\frac{1}{\sqrt{2}}$	$\alpha_- = \pm\mathrm{e}^{\mathrm{i}\phi}\ \alpha_+ = \pm\mathrm{e}^{-\mathrm{i}\phi}\ \beta_+ = \beta_- = 0$		0
	arb.	0	$\pm\frac{\mathrm{i}}{\sqrt{2}}$	$\alpha_- = \alpha_+ = 0\ \beta_+ = \beta_- = \sqrt{2}$		0
5	even	0	0	$\alpha_-\alpha_+ = \frac{1}{2}\ \beta_+\beta_- = \frac{1}{2}\ \alpha_+\beta_- = \pm\frac{1}{2}$		$\sin\frac{\pi}{2L+6}$
5	odd	0	0	$\alpha_-\alpha_+ = \frac{1}{2}\ \beta_+\beta_- = \frac{1}{2}\ \alpha_+\beta_- = \pm\frac{\mathrm{i}}{2}$		0
6	even	0	0	$\alpha_-\alpha_+ = \frac{1}{2}\ \beta_+\beta_- = \frac{1}{2}\ \alpha_+\beta_- = \pm\frac{\mathrm{i}}{2}$		0
6	odd	0	0	$\alpha_-\alpha_+ = \frac{1}{2}\ \beta_+\beta_- = \frac{1}{2}\ \alpha_+\beta_- = \pm\frac{1}{2}$		$\sin\frac{\pi}{2L+4}$
7	even	0	0	$\alpha_-\alpha_+ = \frac{1}{2}\ \beta_+\beta_- = 1\ \alpha_+\beta_- = \pm\frac{1}{\sqrt{2}}$		$\sin\frac{\pi}{2L+4}$
7	odd	0	0	$\alpha_-\alpha_+ = \frac{1}{2}\ \beta_+\beta_- = 1\ \alpha_+\beta_- = \pm\frac{\mathrm{i}}{\sqrt{2}}$		0
8	even	0	0	$\alpha_-\alpha_+ = \frac{1}{2}\ \beta_+\beta_- = 1\ \alpha_+\beta_- = \pm\frac{\mathrm{i}}{\sqrt{2}}$		0
8	odd	0	0	$\alpha_-\alpha_+ = \frac{1}{2}\ \beta_+\beta_- = 1\ \alpha_+\beta_- = \pm\frac{1}{\sqrt{2}}$		$\sin\frac{\pi}{2L+4}$
9	even	0	0	$\alpha_-\alpha_+ = 1\ \beta_+\beta_- = 1\ \alpha_+\beta_- = \pm\sqrt{s}$		$\min(\sin(\frac{\pi}{2L+2} \pm \frac{\mathrm{i}\ln s}{2L+2}))$
	even	0	0	$\alpha_-\alpha_+ = 1\ \beta_+\beta_- = 1\ \alpha_+\beta_- = \pm\frac{1}{\sqrt{s}}$		$\min(\sin(\frac{\pi}{2L+2} \pm \frac{\mathrm{i}\ln s}{2L+2}))$
	even	0	$\pm\frac{\mathrm{i}}{\sqrt{2}}$	$\alpha_- = \alpha_+ = \pm\frac{1}{\sqrt{2}}\ \beta_+ = \beta_- = \pm\sqrt{2}$ $\alpha_+\beta_- = \pm 1$	$s = 1$	$\sin\frac{\pi}{2L+2}$
9	odd	0	0	$\alpha_-\alpha_+ = 1\ \beta_+\beta_- = 1\ \alpha_+\beta_- = \pm\mathrm{i}\sqrt{s}$		$\min(\sin(\frac{\pi}{L+1} \pm \frac{\mathrm{i}\ln s}{2L+2}))$
	odd	0	0	$\alpha_-\alpha_+ = 1\ \beta_+\beta_- = 1\ \alpha_+\beta_- = \pm\frac{\mathrm{i}}{\sqrt{s}}$		$\min(\sin(\frac{\pi}{L+1} \pm \frac{\mathrm{i}\ln s}{2L+2}))$
	odd	0	$\pm\frac{\mathrm{i}}{\sqrt{2}}$	$\alpha_- = \alpha_+ = \pm\frac{1}{\sqrt{2}}\ \beta_+ = \beta_- = \pm\sqrt{2}$ $\alpha_+\beta_- = \pm 1$	$s = -1$	$\sin\frac{\pi}{2L+2}$
10	even	0	0	$\alpha_-\alpha_+ = \frac{s+1}{2}\ \beta_+\beta_- = \frac{s+1}{2s}$ $\alpha_+\beta_- = \pm\frac{(s^{1/2}+s^{-1/2})}{2}$		$\min(\sin\frac{\pi}{2L+2}, \frac{1}{2}(s^{1/2}+s^{-1/2}))$
	even	0	$\pm\frac{\mathrm{i}}{\sqrt{2}}$	$\alpha_- = \alpha_+ = \pm\frac{1}{\sqrt{2}}$ $\beta_+ = \beta_- = \pm\sqrt{\frac{2+s+1/s}{2}}$		$\min(\sin\frac{\pi}{2L+2}, \frac{1}{2}(s^{1/2}+s^{-1/2}))$
10	odd	0	0	$\alpha_-\alpha_+ = \frac{s+1}{2}\ \beta_+\beta_- = \frac{s+1}{2s}$ $\alpha_+\beta_- = \pm\mathrm{i}\frac{(s^{1/2}+s^{-1/2})}{2}$		0
	odd	0	$\pm\frac{\mathrm{i}}{\sqrt{2}}$	$\alpha_- = \alpha_+ = \pm\frac{1}{\sqrt{2}}\ \beta_+ = \beta_- = 0$	$s = -1$	0
11	arb.	0	$\pm\frac{1}{\sqrt{2}}$	$\alpha_- = \alpha_+ = \beta_+ = \beta_- = 0$	$s = -1$	0
12	arb.	$\pm\frac{1}{\sqrt{2}}$	$\pm\frac{1}{\sqrt{2}}$	$\alpha_- = \alpha_+ = \beta_+ = \beta_- = 0$	$s = 1$	0
	arb.	$\mp\frac{\mathrm{i}}{\sqrt{2}}$	$\pm\frac{\mathrm{i}}{\sqrt{2}}$	$\alpha_- = \alpha_+ = 0\ \beta_+ = \beta_- = \pm\sqrt{2}$	$s = 1$	0
13	arb.	$\mp\frac{\mathrm{i}}{\sqrt{2}}$	$\pm\frac{\mathrm{i}}{\sqrt{2}}$	$\alpha_- = \alpha_+ = 0\ \beta_+ = \beta_- = 1$	$s = -1$	0
14	even	$\pm\frac{\mathrm{i}}{\sqrt{2s}}$	$\pm\mathrm{i}\sqrt{\frac{s}{2}}$	$\alpha_- = \alpha_+ = \sqrt{\frac{1+s}{s}}\ \beta_+ = \beta_- = \sqrt{1+s}$		$\min(\sin\frac{\pi}{2L}, \frac{1}{2}(s^{1/2}+s^{-1/2}))$
14	odd	$\pm\frac{1}{\sqrt{2}}$	$\mp\frac{1}{\sqrt{2}}$	$\alpha_- = \alpha_+ = \beta_+ = \beta_- = 0$	$s = -1$	0
15	even	$\pm\frac{1}{\sqrt{2}}$	$\pm\frac{1}{\sqrt{2}}$	$\alpha_- = \alpha_+ = \beta_+ = \beta_- = 0$	$s = -1$	0
15	odd	$\mp\frac{\mathrm{i}}{\sqrt{2s}}$	$\pm\mathrm{i}\sqrt{\frac{s}{2}}$	$\alpha_- = \alpha_+ = \sqrt{\frac{1+s}{s}}\ \beta_+ = \beta_- = \sqrt{1+s}$		$\min(\sin\frac{\pi}{2L}, \frac{1}{2}(s^{1/2}+s^{-1/2}))$
16	arb.	$\pm\frac{1}{\sqrt{2s}}$	$\pm\sqrt{\frac{s}{2}}$	$\alpha_- = \alpha_+ = \beta_+ = \beta_- = 0$		0
	arb.	$\pm\frac{\mathrm{i}}{\sqrt{2}}$	$\mp\frac{\mathrm{i}}{\sqrt{2}}$	$\alpha_- = \alpha_+ = 0\ \beta_+ = \beta_- = \pm(\sqrt{\frac{s}{2}} + \frac{1}{\sqrt{2s}})$		0

such as reflecting the Hamiltonian in the middle of the chain or applying a transformation of the form given by equation (4.3) to the Hamiltonian, are not explicitly listed.

Table 3 should be understood as follows. Let us first comment on the choice of the signs in the cases where we give two alternative signs for the boundary parameters. The signs in the third and fourth columns can always be chosen independently of each other. However, in the upper half of the table, the signs of α_- and α_+ cannot be chosen independently (see e.g. case 2 or 4) whereas in the lower part of the table, they can be chosen independently (e.g. in cases 9 even and 9 odd as indicated by the condition $\alpha_+\beta_- = \pm 1$).

Now we turn to the one-parameter families depending on the parameter s. Here, the conditions (a)–(c) often lead to restrictions for the value of s which are indicated in the fifth column. The choice of α_-, α_+, β_- and β_+ given in the fourth column determines $\alpha_-\beta_+ + \alpha_+\beta_-$. In most of the cases from table 1 the product of all values of Λ_k is positive (or zero), and consequently the sign of $\alpha_-\beta_+ + \alpha_+\beta_-$ multiplied by $(-1)^L$ yields the sign of η. If $\eta < 0$, the ground-state energy of H is given by $E_0(H_{\rm long}) + 2\Lambda_{\rm lowest}$ where $E_0(H_{\rm long})$ can be taken from table 2. If $\eta > 0$, the ground-state energy of H is given by $E_0(H) = E_0(H_{\rm long})$. However, there are some cases where eigenvalues with vanishing real part but non-vanishing imaginary part appear in the spectrum of $H_{\rm long}$. This happens, for example, in case 10 for negative values of s and may in general happen in cases 9, 10, 14 and 15. In these cases, the sign of the product of all eigenvalues is not uniquely defined. Here, it is impossible to decide which of the two vectors $|v^+\rangle$ and $b_{\rm lowest}|v^-\rangle$ corresponds to the ground state of H.

In some of the cases, we always find $\alpha_-\beta_+ + \alpha_+\beta_- = 0$. Here, an additional zero mode appears in the spectrum of $H_{\rm long}$ as already mentioned at the end of section 3. Therefore, the energies of $|v^+\rangle$ and $b_n|v^-\rangle$, where b_n is the creation operator for the additional fermion with energy zero, are the same and the ground-state energy of H is again given by $E_0(H_{\rm long})$. This is also indicated in table 3 in the last column.

13. Guide

In this paper, we have explained how to diagonalize the XX-quantum spin chain of length L with diagonal and non-diagonal boundary terms defined in equation (1.1). Here we give a resumé of our method which the reader may use as a guide on how to use our results. This guide should be seen as a user-friendly cooking recipe. It has two parts, the first deals with the spectrum, the second with the eigenvectors. As one will notice, the guide does not follow the sections in a chronological way.

In order to find the eigenvalues and eigenvectors of H we start by considering a different Hamiltonian $H_{\rm long}$ which is obtained from H by appending two additional sites 0 and $L+1$ (see (1.4)) so that the expression for $H_{\rm long}$ is bilinear in Majorana (Clifford) operators, see equation (2.4). $H_{\rm long}$ can be diagonalized in terms of free fermions, fixing the representation we are working in. The spectrum and the eigenvectors of H in the Fock representation can be retrieved from those found for $H_{\rm long}$ by a projection method described below.

13.1. Eigenvalues of H_{long}

The diagonalization of $H_{\rm long}$ is described in section 2. The spectrum is given in terms of $L+2$ single fermionic energies $2\Lambda_n$ (see (2.16)). The values of Λ_n can be obtained from a $(2L+4) \times (2L+4)$ matrix M (equation (2.11)). Since $M = -M^{\rm t}$, the $2L+4$ eigenvalues of this matrix appear in pairs $\pm\Lambda_n$. The necessary $L+2$ eigenvalues are taken by convention as the values with positive real part. As explained in the text, zero is always an eigenvalue of M. This corresponds to a fermionic zero mode. As long as we consider $H_{\rm long}$, the zero mode

$\Lambda_0 = 0$ appears in the spectrum and the ground state is at least twofold degenerate. As we are going to see, the zero mode does not appear in the spectrum of H; therefore, we are going to call it the spurious zero mode. However, the eigenvectors of M corresponding to the spurious zero mode will be needed in the derivation of the eigenvectors of H.

The eigenvalues of M can be expressed using equation (3.9) in terms of the zeros of a complex polynomial of degree $2L + 4$ (see (4.1)). Note that the variable x in equation (3.9) is related to the variable z in equation (4.1) via $z = x^2$. To find the zeros of the polynomial analytically, we have looked in a systematic way for factorizations of the polynomial into cyclotomic polynomials. We have determined all possible factorizations up to five factors and found some examples for factorizations in six factors. These results are listed in table 1 (the parameters A, B, C, D and E appearing in table 1 are defined by equation (4.2) in terms of the boundary parameters of the Hamiltonian). For the cases where we did not find any factorizations of the polynomial, the zeros of the polynomial and therewith the fermionic energies can still be calculated numerically. Since the polynomial has degree $2L + 4$, this is much easier than a straightforward numerical diagonalization of the Hamiltonian which has dimension $2^L \times 2^L$.

By studying the solutions of the polynomial equation (4.1), we find special L-independent solutions in some cases. They correspond to boundary bound states as will be shown in [23].

The ground-state energy of H_{long} (which is by convention the energy with the smallest real part) is obtained in equation (2.16) by subtracting the Fermi sea. In table 2 we listed the corresponding expressions for the ground-state energies of H_{long} (which are at least twofold degenerate) for the cases where the polynomial factorizes into cyclotomic polynomials. Some properties of the ground-state energies will be discussed in section 14.

In section 6, we give the expressions for the spectrum of M in some of the 'exactly solvable' cases. A list of the ground-state energies of H_{long} for all 'exactly solvable' cases can be found in section 7. Section 8 contains the spectrum of M and the ground-state energy of one example of a Hamiltonian with asymmetric bulk terms which can be treated with the results developed in this paper by using the similarity transformation between the Hamiltonian given by equation (1.1) and that given by (1.2). This transformation changes the boundary parameters according to equation (1.3).

13.2. Eigenvalues and ground-state energy of H

Finding the eigenvalues of the original Hamiltonian H is more involved. As shown in section 9, to find the spectrum H we have to look at an even or an odd number of fermionic excitations with respect to the lowest energy of H_{long}. We disregard the spurious zero mode in the calculation of the number of fermionic excitations. Whether one has an even or an odd number of fermionic excitations in the spectrum of H depends on the value of a parameter η defined by equation (9.5) which is either +1 or -1 (see section 9 for details). We will explain the way it is computed later. If $\eta = +1$, the spectrum of H consists of an even number of fermionic excitations with respect to the ground-state energy of H_{long} and the ground-state energy of H is the same as that of H_{long}. If $\eta = -1$, the eigenvalues of H are given by an odd number of fermionic excitations and the ground-state energy of H is the sum of the ground-state energy of H_{long} and the fermionic energy with the smallest real part which we call $2\Lambda_{\text{lowest}}$.

If on top of the spurious zero mode another fermionic excitation is zero, the ground-state energy of H is non-degenerate and identical to the ground-state energy of H_{long} and the spectrum of H is given by all even and odd combinations of fermionic excitations. If a second fermionic excitation is zero, the whole spectrum of H is twofold degenerate. So in these cases one does not need to calculate the value of η.

At this point we restrict our discussion to the cases where we have derived explicit formulae for the parameter η:

(a) H_{long} (and therewith H) is Hermitian;

(b) H_{long} has no σ^z boundary terms ($\alpha_z = 0 = \beta_z$);

(c) $\alpha_- = \alpha_+$ and $\beta_+ = \beta_-$.

For the other cases this guide is not sufficient since they are much more complicated and we have not obtained simple formulae for the parameter η.

In case (a), η is given by equation (11.13). Notice that only two boundary parameters appear in the expression for η. In cases (b) and (c), the expression for η is given by equation (11.11) in terms of the parameters of the non-diagonal boundary terms and the eigenvalues of M.

13.2.1. Analytical results for the ground-state energy of H. If the Hamiltonian additionally belongs to one of the 'factorizable' cases, the ground-state energy of H can be calculated analytically. These cases are listed in table 3. To calculate the ground-state energy of H for a particular choice of boundary parameters given in the third and fourth column of table 3, one has to proceed as follows. First, one checks the value of $2\Lambda_{\text{lowest}}$ given in the last column. If $2\Lambda_{\text{lowest}} = 0$, the ground-state energy of H is identical to that of H_{long} (which is listed in table 2). In the cases where $2\Lambda_{\text{lowest}} \neq 0$, one has to know the value of η to obtain the ground-state energy of H. This value is obtained by using formula (11.11) in cases (b) and (c) (the values of Λ_n are given by the zeros of the factorized polynomials listed in table 1) and formula (11.13) in case (a).

The fermionic energy with the smallest real part $2\Lambda_{\text{lowest}}$ which has to be added to the ground-state energy of H_{long} if $\eta = -1$ is listed in the last column of table 3. If $\eta = 1$ the ground-state energy of H can be taken directly from table 2.

Many of the exactly solvable cases depend on an arbitrary free parameter s (see tables 1 and 3). In table 3, these s-dependent cases can be separated into two categories. For cases 11–13 and for some choices of the parameters in cases 9, 10, 14 and 15, the conditions (a)–(c) fix the parameter s to some particular value which can be found in column 5 of table 3. For cases 9, 10, 14–16 there are also possible choices of the boundary parameters where this is not the case. In examples 9, 10, 14 and 15 it may happen that one cannot make a definite statement about the value of η, if s is chosen in such a way that the s-dependent eigenvalue of M has a vanishing real part, but a non-vanishing imaginary part. The reason lies in the fact that our convention to choose the fermionic energies as those with positive real part becomes ambiguous in this case.

13.2.2. Numerical calculation of the ground-state energy of H. Even if the Hamiltonian one is interested in does not belong to one of the factorizable cases, but fulfils conditions (a), (b) or (c), one can still use formulae (11.13) and (11.11) to decide what the ground state of H is. If H is Hermitian, η can be read off directly from (11.13); in cases (b) and (c) one additionally needs the spectrum of M to compute the value of η (see (11.11)). The eigenvalues of M can be calculated numerically by solving the polynomial equation (4.1) or by diagonalizing M numerically. Inserting them into equation (2.16) yields the ground-state energy of H_{long}.

13.3. Eigenvectors of H_{long}, H and M

Up to now we have described how to find the eigenvalues and the ground-state energies for H_{long} and for H. Let us now turn to the eigenvectors.

The eigenvectors of H_{long} are given in a fermionic Fock representation (compare equation (2.16)). The eigenvectors of H are given in the same Fock representation; however, they all lie either in the even or the odd part of the Fock space where we again do not count the spurious zero mode. If the value of η is +1, the ground state of H corresponds to $|v^+\rangle$ (see equation (9.3)) and all excited states are of the form given in equation (9.6). If $\eta = -1$, the ground state of H corresponds to $b_{\text{lowest}}|v^-\rangle$ where $|v^-\rangle$ is also defined in equation (9.3) and b_{lowest} is the creation operator corresponding to the fermion energy with the smallest real part. For the exactly solvable cases it can be read off table 3. The excited states are described by equation (9.7).

In section 10, we describe how to calculate expectation values of σ-operators. For this calculation, one can either transform the expression for the eigenstates of H in the spin representation or, alternatively, one can transform the expression for the σ-operators into the fermionic (Fock) representation. We have chosen the second possibility. The transformation from the σ-operators to the fermionic operators a_k and b_k is given in equations (2.3) and (10.3) where the $(\phi_k^{\pm})_j^{\mu}$ are the components of the eigenvectors of M defined by (2.13) (where we use the notation fixed by (2.9)). Thus, to use this transformation one needs to know the eigenvectors of M. We will now describe how to find them analytically in the cases where the zeros of the polynomial are known, following the method described in section 3. One first solves equation (3.17) to express φ_1 as a function of $\bar{\varphi}_1$, where the coefficients Ω_{ij} with $i, j = 1, 2$ are given by equations (3.18)–(3.21). If $x \neq \mathrm{i}$, the solution for φ_1 is inserted in equations (3.11)–(3.14), and the results for the coefficients a, b, f and g used in equation (3.8) for $x \neq 1$ respectively (3.23) for $x = 1$ yield expressions for φ_j and $\bar{\varphi}_j$. The entries of the eigenvector $\phi^{\pm}$ are then given by (3.24) in terms of φ_j and $\bar{\varphi}_j$. In this notation, they still depend on the variable x.

The values of x are obtained as solutions of the polynomial equation (4.1). The polynomial is given in the variable $z = x^2$. The eigenvectors for the eigenvalues Λ_n with positive real part and $x_n \neq \mathrm{i}$ are obtained by choosing a square root $x_n = \sqrt{z_n}$ for each zero $z_n \neq \pm 1$ of the polynomial (such that the real part of x_n is positive). Observe that due to the quadratic relation between Λ_n and x_n (equation (3.9)) the values x_n and $1/x_n$ lead to the same eigenvalue and to the same eigenvector.

For the eigenvectors corresponding to the eigenvalues Λ_n with negative real part one takes $x_n = -\sqrt{z_n}$. The last free parameter $\bar{\varphi}_1$ is fixed by the normalization conditions given by equation (2.20). Equations (2.20) and (2.21) are equivalent to the anticommutation relations for the fermionic operators.

For $x_n = \mathrm{i}$ the equations (3.3)–(3.7) have to be solved in a different way using the ansatz given by (3.8) for φ_j and $\bar{\varphi}_j$. Details of this calculation as well as a derivation of the conditions for the appearance of additional zero modes on top of the spurious zero mode in the spectrum of H_{long} can be found in the appendix.

13.4. One- and two-point functions of the σ^x-operators

If no σ^z-boundary terms are present in the Hamiltonian or if the condition $\alpha_- = \alpha_+$ and $\beta_+ = \beta_-$ is met, we obtained formulae for the one- and two-point functions of the σ_j^x-operator for both chains H and H_{long}. For H_{long}, we considered the ground states given by the eigenstates of σ_0^x and σ_{L+1}^x. Remember that H_{long} has a twofold degenerate ground state due to the spurious zero mode. In the fermionic language, this corresponds to a vacuum, $|\text{vac}\rangle$, and an excited zero mode, $|0\rangle$. Due to the symmetry that H_{long} commutes with σ_0^x and σ_{L+1}^x we can pick out the two ground states $|v^{\pm}\rangle =$

$|\mathrm{vac}\rangle \pm |0\rangle$ (see (9.3)) as eigenstates of σ_0^x and σ_{L+1}^x. As far as H is concerned, its ground state is given either by $|v^+\rangle$ or by $b_{\mathrm{lowest}}|v^-\rangle$, where b_{lowest} is the creation operator of the fermion corresponding to the energy with the smallest real part as explained earlier.

The one-point functions of the σ_j^x-operator are non-trivial due to the presence of the non-diagonal boundary terms. Without them, they would be zero which is a well known fact from the XX-chain.

The one- and two-point functions are, up to a factor, Pfaffians (see (10.1), (10.2) and (10.5)) of the matrix $\mathbf{A}$ given by equation (10.6). If no σ^z-boundary terms are present, we can further reduce this expression to a determinant as given by equation (10.11). If $\alpha_- = \alpha_+$ and $\beta_+ = \beta_-$, the determinant is given by (10.14). These simplifications are possible because some of the so-called basic contractions of pairs of the form given by (10.8) vanish due to the relations (2.40) and (2.42) obtained in section 2. To determine the ground state of H, we use the results of this calculation to determine the magnetization $\langle v^+|\sigma_{L+1}^x|v^+\rangle$ in section 11 to find the value of the parameter η as given by (11.11).

Our calculation with slight modifications also applies to expectation values of the σ_j^x-operator with respect to excited states. This is explained in the last paragraph of section 10.

13.5. List of the results which are going to be used in the following two papers

Here we give a list of results that we will use in the following two papers.

• Second paper [23]. In order to calculate expectation values of the σ_j^z-operator and the σ_j^x-operator for arbitrary position j and lattice length L, we need:

(i) the transformation from the σ-operators to the fermionic operators ((2.3) and (10.3));

(ii) the eigenvectors of M (see section 3) and the roots of the polynomial (4.1);

(iii) the expressions for the eigenstates of H in the Fock representation ((9.6), (9.7) and (9.3)) and the value of the parameter η defined by equation (9.5);

(iv) the formulae for the one- and two-point correlation functions of σ_j^x derived in section 10.

• Third paper [24].

(i) For the calculation of the excitation spectrum of H in the limit of large L we need the polynomial equation (4.1) and the projection mechanism (see section 9).

(ii) For the expressions of the ground-state energies in the exactly solvable cases in the limit of large L we need the results of tables 2 and 3.

(iii) For the construction of the magnetic charge operator, we need the eigenvectors of M (and therewith the roots of the polynomial, see earlier).

14. Discussion

14.1. Observations on the expressions for the ground-state energies

Up to now we have described how to find the eigenvalues, the ground-state energies and the eigenvectors for H_{long} (equation (1.4)) and for H (equation (1.1)). We now turn to the discussion of the results of our analytical calculations for the cases where the polynomial (equation (4.1)) can be factorized into cyclotomic polynomials. The expressions of the ground-state energies of H_{long} and of H are given in terms of trigonometric functions only (see tables 2 and 3). It is remarkable that they appear in spite of non-diagonal boundary terms in the Hamiltonians. This reflects the integrability of the model.

Furthermore, notice that for the one-parameter families of exact solutions corresponding to cases 10–16 from table 2 (where the free parameter is called s) the ground-state energy has an L-independent (but s-dependent) term which appears additively to the L-dependent part of the ground-state energy. We will show in [23] that these L-independent contributions to the ground-state energy of H are related to boundary bound states.

In some special situations, which only appear for non-Hermitian Hamiltonians, the expressions for the ground-state energy of H exhibit a rather peculiar behaviour with respect to variations of L. Namely, considering one of the cases 10, 14 and 15 and choosing the parameter s in such a way that $\eta = -1$, one observes that for L less than a limiting length L_{limit} (which depends on s) the fermionic energy $2\,\Lambda_{\text{lowest}}$ (which has to be added to the ground-state energy of H_{long} to obtain the ground-state energy of H) is given by twice the L-independent expression that appears in the ground-state energy of H_{long}, but with opposite sign (see table 3). Therefore, this term appears with different sign in the expression for the ground-state energy of H than in the expression for the ground-state energy of H_{long}. However, if L is larger than L_{limit}, a level crossing in the fermionic spectrum appears and another L-dependent fermionic energy becomes smaller than the L-independent energy from before. Then this L-dependent fermionic energy has to be added to the ground state of H_{long} instead of the L-independent term from before, and the L-independent part no longer switches its sign when going from the ground-state energy of H_{long} to that of H.

Now we discuss the degeneracies in the spectrum of H. Degeneracies may appear due to doubly degenerate fermionic energies. In the cases where the polynomial can be factorized into cyclotomic polynomials, twofold degenerate fermionic energies can be identified by quadratic factors appearing in the factorized form of the polynomial (see table 1). Notice that this observation does not apply to the quadratic factors of the form $(1-z)^2$ since the polynomial $p(z)$ given by equation (4.1) has to be divided by this term. In the case where the spectrum of H consists of an odd number of fermionic excitations, twofold degenerate fermionic energies also lead to a twofold degenerate ground state. The degeneracies in the spectrum of H are also reflected in the partition functions in [24].

14.2. Open questions

Some questions could not be clarified within the framework of this paper.

(a) It is not clear whether table 1 from section 5 shows all possible cases where the polynomial factorizes into six or more factors given by cyclotomic polynomials. Perhaps it is also possible to find different factorizations of the polynomial for other boundary parameters which also allow us to compute all zeros analytically.

(b) From table 3 one sees that two Hamiltonians may have different boundary terms and still have the same spectrum (given by the zeros of the same polynomial), for example in case 2 where the Hamiltonian H with $\alpha_-\alpha_+ = 1$ and $\beta_+ = \beta_- = \alpha_z = \beta_z = 0$ has the same spectrum as the Hamiltonian with boundary parameters $\beta_z = \frac{1}{\sqrt{2}}, \alpha_z = 0, \alpha_- = \frac{1}{\sqrt{2}}\mathrm{e}^{\mathrm{i}\phi}, \alpha_+ = \frac{1}{\sqrt{2}}\mathrm{e}^{-\mathrm{i}\phi}, \beta_+ = \beta_- = 0$. This fact gives rise to unknown similarity transformations which remain to be made explicit.

(c) For the exactly solvable one-parameter families 10, 14 and 15 with free parameter s we observed a surprising behaviour of the expression of the ground-state energy of H in the case where the parameter $\eta = -1$. Namely, by increasing the lattice length L and reaching a certain value L_{limit} which is given in terms of s, the L-independent contribution to the ground-state energy suddenly switches its sign. The physical origin of this phenomenon is not clear.

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Appendix. Appearance of fermionic zero modes in the spectrum of H_{long}

In this appendix, we show how to find the eigenvectors of the matrix M corresponding to the eigenvalue zero. This procedure will provide conditions for the boundary parameters which are equivalent to the existence of additional zero modes on top of the spurious zero mode. These conditions are already mentioned without proof in section 3.

One might guess that the conditions on the boundary parameters we obtain by constructing the eigenvectors are already contained in the polynomial given by equation (4.1). We will see that this is indeed the case, if we only consider Hermitian boundary terms. In the general, non-Hermitian case this is not true. The polynomial might have more zeros corresponding to eigenvalues $\lambda = 0$ of the matrix M than the number of eigenvectors that can be constructed. Therefore, in this case, M is not diagonalizable.

We are first going to deal with the explicit construction of the eigenvectors. Afterwards we will consider the polynomial equation (4.1).

A.1. Construction of eigenvectors

According to equation (3.9), $\lambda = 0$ corresponds to $x = \pm\mathrm{i}$. So we solve the boundary equations (3.4)–(3.7) using the solution of the bulk equations (3.3) given by (3.8) with $x = \mathrm{i}$, i.e.

$$\varphi_j = a\mathrm{i}^j + b\mathrm{i}^{-j} \qquad \bar{\varphi}_j = g(-\mathrm{i})^j + f(-\mathrm{i})^{-j} \tag{A.1}$$

where $0 < j < L + 1$. This can now be used to rewrite the boundary equations in terms of a, b, g, f and $\varphi_0, \bar{\varphi}_0, \varphi_{L+1}, \bar{\varphi}_{L+1}$. Introducing the new parameters

$$r_\alpha^\pm = (\tfrac{1}{\sqrt{2}} \pm \mathrm{i}\alpha_z) \qquad r_\beta^\pm = (\tfrac{1}{\sqrt{2}} \pm \mathrm{i}\beta_z) \tag{A.2}$$

we obtain from the left boundary

$$\varphi_0 = \bar{\varphi}_0 \tag{A.3}$$

$$\alpha_-(a - b) = \alpha_+(f - g) \tag{A.4}$$

$$r_\alpha^+ a + r_\beta^+ b - \alpha_+\varphi_0 = 0 \tag{A.5}$$

$$r_\beta^+ g + r_\alpha^+ f - \alpha_-\varphi_0 = 0. \tag{A.6}$$

The equations from the right boundary give

$$(-1)^L r_\beta^- a - r_\beta^+ b + \mathrm{i}^{L+1}\beta_+\varphi_{L+1} = 0 \tag{A.7}$$

$$r_\beta^+ g - (-1)^L r_\beta^- f + \mathrm{i}^{L+1}\beta_-\varphi_{L+1} = 0 \tag{A.8}$$

$$\beta_+(g + (-1)^L f) = -\beta_-(b + (-1)^L a) \tag{A.9}$$

$$\varphi_{L+1} = -\bar{\varphi}_{L+1}. \tag{A.10}$$

Since $\bar{\varphi}_0$ and $\bar{\varphi}_{L+1}$ appear only in equations (A.3) and (A.10), we have to solve the homogeneous system of six linear equations given by (A.4)–(A.9) for the six unknowns $a, b, f, g, \varphi_0, \varphi_{L+1}$. The vector components $\bar{\varphi}_0$ and $\bar{\varphi}_{L+1}$ can then be directly read off from equation (A.3)

respectively (A.10). To have non-trivial solutions for the 6×6 system of equations (A.4)–(A.9) the determinant of the corresponding 6×6 matrix has to vanish. This is equivalent to a condition on the boundary parameters α_+, α_-, β_+, β_-, i.e.

$$\alpha_+\beta_- + \alpha_-\beta_+ = 0. \tag{A.11}$$

At this point, it is not obvious how many solutions of the equations (A.4)–(A.9) may exist. Thus we are going to solve them explicitly. In order to do this, we will treat (A.5)–(A.8) and (A.4) and (A.9) separately. We first solve (A.5)–(A.8) for a, b, f, g and then check for consistency with (A.4) and (A.9).

Equations (A.5) and (A.7) and (A.6) and (A.8) can be rewritten as

$$R_{ab}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \alpha_+\varphi_0 \\ -\mathrm{i}^{L+1}\beta_+\varphi_{L+1} \end{pmatrix} \qquad R_{gf}\begin{pmatrix} g \\ f \end{pmatrix} = \begin{pmatrix} \alpha_-\varphi_0 \\ -\mathrm{i}^{L+1}\beta_-\varphi_{L+1} \end{pmatrix} \tag{A.12}$$

where the 2×2 matrices R_{ab} and R_{gf} are given by

$$R_{ab} = \begin{pmatrix} r_\alpha^+ & r_\beta^+ \\ (-1)^L r_\beta^- & -r_\beta^+ \end{pmatrix} \qquad R_{gf} = \begin{pmatrix} r_\beta^+ & r_\alpha^+ \\ r_\beta^+ & (-1)^{L+1} r_\beta^- \end{pmatrix}. \tag{A.13}$$

The determinants of R_{ab} and R_{gf} have the same values and are given in terms of α_z, β_z by

$$\det R_{ab} = \det R_{gf} = \begin{cases} 2\beta_z\alpha_z - 1 & \text{for } L \text{ even} \\ -\sqrt{2}\mathrm{i}(\alpha_z + \beta_z) & \text{for } L \text{ odd.} \end{cases} \tag{A.14}$$

Once we know the general solution of equation (A.12), we only have to verify which specific solutions simultaneously solve (A.4) and (A.9). Solving equation (A.12) one has to distinguish two cases: (1) $\det R_{ab} \neq 0$, (2) $\det R_{ab} = 0$. Let us first deal with case (1).

If $\det R_{ab} \neq 0$ the matrices R_{ab} and R_{gf} can be inverted in order to solve (A.12). Doing this we obtain

$$a = \frac{-1}{\det R_{ab}}(\alpha_+ r_\beta^+\varphi_0 - \mathrm{i}^{L+1}\beta_+ r_\beta^+\varphi_{L+1}) \tag{A.15}$$

$$b = \frac{-1}{\det R_{ab}}((-1)^L\alpha_+ r_\beta^-\varphi_0 + \mathrm{i}^{L+1}\beta_+ r_\alpha^+\varphi_{L+1}) \tag{A.16}$$

$$g = \frac{-1}{\det R_{ab}}((-1)^L\alpha_- r_\beta^-\varphi_0 - \mathrm{i}^{L+1}\beta_- r_\alpha^+\varphi_{L+1}) \tag{A.17}$$

$$f = \frac{-1}{\det R_{ab}}(\alpha_- r_\beta^+\varphi_0 + \mathrm{i}^{L+1}\beta_- r_\beta^+\varphi_{L+1}). \tag{A.18}$$

Substituting this into equation (A.4) gives

$$(\alpha_+\beta_- + \alpha_-\beta_+)\varphi_{L+1} = 0 \tag{A.19}$$

whereas (A.9) leads to

$$(\alpha_+\beta_- + \alpha_-\beta_+)\varphi_0 = 0. \tag{A.20}$$

Thus, if equation (A.11) is satisfied and if $\det R_{ab} \neq 0$, we obtain two eigenvectors of M corresponding to the eigenvalue $\lambda = 0$ on top of the spurious zero mode because φ_0 and φ_{L+1} can be chosen independently of each other.

Let us now turn to case (2), i.e. $\det R_{ab} = 0$. Because this condition gives different conditions on the non-diagonal boundary terms for L even and L odd, respectively (see (A.14)), we discuss these cases separately.

We will first turn to the case where L is odd. Here we have $\alpha_z = -\beta_z$ which can be read off from equation (A.14). Using this in (A.13), we can rewrite (A.12) as follows:

$$\alpha_+\varphi_0 = \mathrm{i}^{L+1}\beta_+\varphi_{L+1} \qquad \alpha_-\varphi_0 = -\mathrm{i}^{L+1}\beta_-\varphi_{L+1} \tag{A.21}$$

$$\alpha_+\varphi_0 = r_\beta^- a + r_\beta^+ b \qquad \alpha_-\varphi_0 = r_\beta^- f + r_\beta^+ g. \tag{A.22}$$

For L even we have, according to equation (A.14), $\alpha_z = 1/2\beta_z$. Using this equality, (A.12) reads

$$\sqrt{2}\beta_z\alpha_+\varphi_0 = \mathrm{i}^L\beta_+\varphi_{L+1} \qquad \sqrt{2}\beta_z\alpha_-\varphi_0 = -\mathrm{i}^L\beta_-\varphi_{L+1} \tag{A.23}$$

$$\mathrm{i}\sqrt{2}\beta_z\alpha_+\varphi_0 = r_\beta^+ b - r_\beta^- a \qquad \mathrm{i}\sqrt{2}\beta_z\alpha_-\varphi_0 = r_\beta^+ g - r_\beta^- f. \tag{A.24}$$

Note that at least one of the parameters r_β^-, r_β^+ is different from zero. Thus, equations (A.22) and (A.24) can be solved either for a and f or for b and g, respectively. Note also that, due to (A.21) and (A.23), φ_0 and φ_{L+1} are no longer independent of each other, if one of the parameters α_+, α_-, β_+, β_- is different from zero in contrast to case (1).

If all of the parameters α_+, α_-, β_+, β_- are vanishing, equation (A.21) respectively (A.23) are satisfied automatically. The same holds for equations (A.4) and (A.9). Thus we simply have to solve equations (A.22) and (A.24) yielding

$$a = (-1)^L\frac{r_\beta^+}{r_\beta^-}b \qquad f = (-1)^L\frac{r_\beta^+}{r_\beta^-}g \qquad \text{for } r_\beta^- \neq 0 \tag{A.25}$$

$$b = (-1)^L\frac{r_\beta^-}{r_\beta^+}a \qquad g = (-1)^L\frac{r_\beta^-}{r_\beta^+}f \qquad \text{for } r_\beta^+ \neq 0. \tag{A.26}$$

Since, on the one hand, the parameters a and f or b and g, respectively, and, on the other, the two vector components φ_0, φ_{L+1} can be chosen independently we obtain a set of four eigenvectors corresponding to the eigenvalue $\lambda = 0$ on top of the spurious zero mode.

If one of the parameters $\alpha_+, \alpha_-, \beta_+, \beta_-$ is different from zero we may solve equations (A.22) and (A.24) for a and f or b and g, respectively, and use the result in equation (A.4) to obtain

$$\alpha_- b = \alpha_+ g \qquad \text{for } r_\beta^- \neq 0 \tag{A.27}$$

$$\alpha_- a = \alpha_+ f \qquad \text{for } r_\beta^+ \neq 0. \tag{A.28}$$

Additionally using equation (A.21) respectively (A.23), we obtain from equation (A.9)

$$\beta_+ g = -\beta_- b \qquad \text{for } r_\beta^- \neq 0 \tag{A.29}$$

$$\beta_+ f = -\beta_- a \qquad \text{for } r_\beta^+ \neq 0. \tag{A.30}$$

Due to condition (A.11), it is always possible to solve equations (A.27)–(A.30) and (A.21) respectively (A.23) by leaving two variables undetermined. The remaining four unknowns can then be given in terms of these two. This allows the construction of two further eigenvectors corresponding to the eigenvalue $\lambda = 0$.

For instance, let us assume $\alpha_+ \neq 0$, $r_\beta^- \neq 0$ and L odd. Equation (A.21) is then solved by $\varphi_0 = \mathrm{i}^{L+1}(\beta_+/\alpha_+)\varphi_{L+1}$, whereas (A.27) and (A.29) are solved by $g = (\alpha_-/\alpha_+)b$. The parameters a and f are then fixed by equation (A.22). Thus a, f, g, φ_0 are given in terms of b and φ_{L+1}, which can be chosen independently.

Let us briefly summarize the results of this section. We have looked for eigenvectors corresponding to the eigenvalue zero. At this point we want to remind the reader that there always exist at least two eigenvectors corresponding to the eigenvalue zero, namely those which are related to the spurious zero mode. We found exactly two further eigenvectors corresponding to the eigenvalue zero of M if and only if one of the two following conditions is satisfied:

(i) $\alpha_+\beta_- + \beta_+\alpha_- = 0$ and $\beta_z \neq 1/2\alpha_z$ for L even respectively $\alpha_z \neq -\beta_z$ for L odd;

(ii) $\alpha_+\beta_- + \beta_+\alpha_- = 0$ and at least one of the parameters $\alpha_\pm$, $\beta_\pm$ is different from zero.

There exist four further eigenvectors corresponding to the eigenvalue zero of M if and only if

(i) $\alpha_\pm = \beta_\pm = 0$ and $\beta_z = 1/2\alpha_z$ for L even respectively $\alpha_z = -\beta_z$ for L odd.

There are no other possibilities of having further eigenvectors corresponding to the eigenvalue zero.

A.2. Zeros of the polynomial at $z = -1$

In this subsection we consider the polynomial equation (4.1) in order to check whether the matrix M may have more eigenvalues $\lambda = 0$ than the number of eigenvectors that can be constructed. Since in general M is non-Hermitian, this may indeed be the case. For Hermitian M, i.e. Hermitian boundary conditions, we will recover the conditions on the boundary terms which we already obtained in the previous section.

Since the polynomial equation is given in terms of the variable $z = x^2$, an additional eigenvalue $\lambda = 0$ on top of the spurious zero mode corresponds to a root of the polynomial at $z = -1$ (see (3.9)). The necessary condition to have at least one eigenvalue $\lambda = 0$ on top of the spurious zero mode therefore translates to

$$q(-1) = 0$$
$$\Leftrightarrow D = 1 + A + B + 2C \tag{A.31}$$
$$\Leftrightarrow \alpha_-\beta_+ + \alpha_+\beta_- = 0 \tag{A.32}$$

where the parameters A, B, C, D and E are defined by equations (4.2). These zeros will always appear in pairs since with z also $1/z$ is a zero of $q(z)$. In order to find a condition for the existence of a root at $z = -1$ with higher multiplicity than two, we have to consider the second derivative of $q(z)$. Using equation (A.31) we obtain for even L

$$\partial_z^2 p(z)|_{z=-1} = 0$$
$$\Leftrightarrow 2(E-1)^2 + (3 + 2A + B + 2C)L - CL^2 = 0 \tag{A.33}$$

whereas for odd L we get

$$1 - C - B + 4E + (3 + 2A + B + 2C)L - CL^2 = 0. \tag{A.34}$$

Let us now consider equations (A.32)–(A.34) for the case of Hermitian boundaries. Then equation (A.32) implies that at least one of the parameters $\alpha_+ = \alpha_-^*$ or $\beta_+ = \beta_-^*$ is equal to zero. Without loss of generality, we may assume that $\alpha_+ = 0$. This implies immediately $C = 0$ and $3 + 2A + B = 2|\beta_+|^2(1 + 2\alpha_z^2)$. Using equation (A.33) we obtain for L even

$$2|\beta_+|^2(1 + 2\alpha_z^2) = -\frac{2(2\alpha_z\beta_z - 1)^2}{L}. \tag{A.35}$$

Since this equality can only be valid if the right-hand side and the left-hand side vanish simultaneously, we conclude that in the Hermitian case further zeros at $z = -1$ only exist if

$$\alpha_+ = \beta_+ = 0 \qquad \alpha_z = \frac{1}{2\beta_z}. \tag{A.36}$$

From equation (A.34) we get for L odd

$$2|\beta_+|^2(1 + 2\alpha_z^2) = -\frac{4(\beta_z + \alpha_z)^2}{L} \tag{A.37}$$

which can only be satisfied if

$$\alpha_+ = \beta_+ = 0 \qquad \alpha_z = -\beta_z. \tag{A.38}$$

Further conditions for the existence of more than four zeros at $z = -1$ can be derived in the same manner as equation (A.33) and equation (A.34), respectively. Solving (A.33) and (A.34) for A and calculating the fourth derivative of $p(z)$ at $z = -1$ gives the conditions

$$4 - 8E + E^2 + 12L(1 - E^2) + L^2(2E^2 - 3B - 4C + 8E + 5) + L^4C = 0 \tag{A.39}$$

for L even and

$$C + 8E + B + 6E^2 + 5 + 12L(1 - E^2) + L^2(7 - 2C - 8E - B + 6E^2) + L^4C = 0 \tag{A.40}$$

for L odd, respectively. Using equations (A.36) in (A.39) gives

$$\left(\sqrt{2}\beta_z + \frac{1}{\sqrt{2}\beta_z}\right)^2 = 0 \tag{A.41}$$

whereas substitution of (A.38) into (A.40) yields

$$-2\beta_z^2 = \frac{1+L}{L-1}. \tag{A.42}$$

Since neither equation (A.41) nor (A.42) can be satisfied by any $\beta_z \in \mathbb{R}$ we conclude that in the Hermitian case we have at most four zeros at $z = -1$. It is no surprise that for Hermitian boundaries the conditions on the boundary parameters obtained in this subsection are equivalent to those of the previous subsection. However, if M is non-Hermitian, the conditions derived in this subsection have more solutions than those of the previous section. Therefore, it may happen that the polynomial has more zeros corresponding to an eigenvalue $\lambda = 0$ than the number of eigenvectors that can be constructed. This implies that M is non-diagonalizable for certain choices of boundary terms.

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