Spectrum of a duality-twisted Ising quantum chain

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Abstract. The Ising quantum chain with a peculiar twisted boundary condition is considered. This boundary condition, first introduced in the framework of the spin-1/2 XXZ Heisenberg quantum chain, is related to the duality transformation, which becomes a symmetry of the model at the critical point. Thus, at the critical point, the Ising quantum chain with the duality-twisted boundary is translationally invariant, similar as in the case of the usual periodic or antiperiodic boundary conditions. The complete energy spectrum of the Ising quantum chain is calculated analytically for finite systems, and the conformal properties of the scaling limit are investigated. This provides an explicit example of a conformal twisted boundary condition and a corresponding generalised twisted partition function.

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Recently, there has been a lot of interest in generalised twisted partition functions of conformal field theory [1, 2, 3, 4] and the corresponding conformal twisted boundary conditions in solvable lattice models of statistical mechanics [5]. Examples of such boundary conditions leading to the appearance of "exotic" spinor operators in the corresponding conformal field theory had previously been considered for quantum spin chains, in particular for the Ising and 3-state Potts quantum chains [6, 7]. In these cases, the boundary conditions were derived from a mapping [8, 9, 10, 11, 12, 6] between these models with N sites and the spin-1/2 XXZ Heisenberg model with twisted boundary conditions, which for an even number of sites $2N$ yields the "usual" twisted boundary conditions [8, 10], such as antiperiodic boundary conditions for the Ising quantum chain, and results in rather exotic boundary terms when considered for an odd number of sites $2N-1$ [6]. The corresponding boundary conditions still allow for translational symmetry, but only at the critical point. The corresponding symmetry for the Ising and Potts models was identified as duality, which maps the Ising Hamiltonian of the ordered phase onto that of the disordered phase and vice versa. It becomes a proper symmetry at the critical point, and the corresponding boundary terms and generalised translation and parity operators were analysed in [6, 7] by means of an algebraic approach [13].

The conformal partition function corresponding to this duality twisted boundary condition was derived in [6] from that of the twisted XXZ Heisenberg spin chain [14]. However, the spectrum of the duality-twisted Ising quantum chain itself has never been calculated explicitly. In fact, using the standard free-fermion approach [15], it is possible to obtain the complete spectrum even for finite chains. This is the purpose of this

Letter. The calculation proceeds along the same path as for Ising quantum chains with "generalised defects" [16], as the boundary terms are actually rather similar. However, the defects considered in [16], albeit featuring rather general couplings of the last and the first spin in the chain, did not include the duality-twisted boundary considered here. For comparison, we treat the usual periodic and antiperiodic boundary conditions in the same way.

Consider an Ising quantum spin chain consisting of N sites, so the Hilbert space is $\mathcal{H}_N = (\mathbb{C}^2)^{\otimes N} \cong \mathbb{C}^{2^N}$. We introduce local spin operators, acting at site j, by

$$\sigma_j^w = \left(\bigotimes_{k=1}^{j-1} \mathbb{I}\right) \otimes \sigma^w \otimes \left(\bigotimes_{k=j+1}^{N} \mathbb{I}\right), \tag{1}$$

where w stands for x, y and z, and $\mathbb{I}$ denotes the unit operator. In the canonical basis, the spin operators σ^w are represented by the Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2}$$

and $\mathbb{I}$ is the 2×2 unit matrix.

The critical Ising quantum chain with periodic $(+)$ and antiperiodic $(-)$ boundary conditions is defined by the Hamiltonians

$$H^{(\pm)} = -\frac{1}{2}\left(\sum_{j=1}^{N-1} \sigma_j^x \sigma_{j+1}^x + \sum_{j=1}^{N} \sigma_j^z \pm \sigma_N^x \sigma_1^x\right). \tag{3}$$

The Ising quantum chain is related to the transfer matrix of the classical zero-field square-lattice Ising model at the critical temperature through an anisotropic limit. The normalisation factor is chosen such that the fermion velocity in the scaling limit is equal to unity. The duality-twisted Ising quantum chain is given by [6, 7]

$$H^{(\mathrm{d}\pm)} = -\frac{1}{2}\left(\sum_{j=1}^{N-1} \sigma_j^x \sigma_{j+1}^x + \sum_{j=1}^{N-1} \sigma_j^z \pm \sigma_N^y \sigma_1^x\right). \tag{4}$$

Note that, besides the coupling between σ_N^y and σ_1^x, the Hamiltonians (4) and (3) also differ in the diagonal terms, as there is no operator σ_N^z in (4). This is also the reason why such boundary terms were not considered as a "generalised defect" in [16]. Because the generalised parity transformation for the duality-twisted Hamiltonian maps the two signs at the boundary onto each other [7], and since the two Hamiltonians are related by complex conjugation, they have the same spectrum, and the momenta of the eigenstates differ by a sign.

The Hamiltonians $H^{(\pm)}$ and $H^{(\mathrm{d}\pm)}$ commute with the operator

$$Q = (\sigma^z)^{\otimes N} = \prod_{j=1}^{N} \sigma_j^z, \tag{5}$$

so they have a global C_2 symmetry. We denote the corresponding projectors by

$$P_\pm = \frac{1}{2}\left(\mathbb{I}_N \pm Q\right), \tag{6}$$

where $\mathbb{I}_N = \mathbb{I}^{\otimes N}$ is the identity operator on $\mathcal{H}_N$. In addition, they commute with properly defined translation operators, which take the boundary condition into account, see [13, 6, 7] for details.

In order to obtain local boundary conditions in the fermionic language, we play the usual trick and pass to "mixed-sector" Hamiltonians [17] defined as

$$\tilde{H}^{(\pm)} = H^{(\pm)} P_+ + H^{(\mp)} P_-, \tag{7}$$

$$\tilde{H}^{(\mathrm{d}\pm)} = H^{(\mathrm{d}\pm)} P_+ + H^{(\mathrm{d}\mp)} P_-. \tag{8}$$

Performing a Jordan-Wigner transformation [15]

$$c_k = \left(\prod_{j=1}^{k-1} \sigma_j^z \right) \sigma_k^-, \qquad c_k^\dagger = \left(\prod_{j=1}^{k-1} \sigma_j^z \right) \sigma_k^+, \tag{9}$$

we rewrite $\tilde{H}^{(\pm)}$ and $\tilde{H}^{(\mathrm{d}\pm)}$ as bilinear expressions in the fermionic creation and annihilation operators $c_k^\dagger$ and c_k,

$$\tilde{H} = \frac{N}{2}\mathbb{I}_N + \sum_{j,k=1}^{N} \left[D_{j,k} c_j^\dagger c_k + \frac{1}{2}\left(E_{j,k} c_j^\dagger c_k^\dagger + E_{k,j}^* c_j c_k \right) \right], \tag{10}$$

where the $N \times N$ matrices D and E depend on the boundary conditions

$$\begin{aligned} 2D_{j,k}^{\pm} = & -2\delta_{j,k} + \delta_{j+1,k}(1-\delta_{j,N}) + \delta_{j,k+1}(1-\delta_{k,N}) \\ & \mp \delta_{j,1}\delta_{k,N} \mp \delta_{j,N}\delta_{k,1}, \end{aligned} \tag{11}$$

$$2E_{j,k}^{\pm} = \delta_{j+1,k}(1-\delta_{j,N}) - \delta_{j,k+1}(1-\delta_{k,N}) \pm \delta_{j,1}\delta_{k,N} \mp \delta_{j,N}\delta_{k,1}, \tag{12}$$

$$\begin{aligned} 2D_{j,k}^{\mathrm{d}\pm} = & -2\delta_{j,k}(1-\delta_{j,N}) + \delta_{j+1,k}(1-\delta_{j,N}) + \delta_{j,k+1}(1-\delta_{k,N}) \\ & \mp \mathrm{i}\,\delta_{j,1}\delta_{k,N} \pm \mathrm{i}\,\delta_{j,N}\delta_{k,1}, \end{aligned} \tag{13}$$

$$2E_{j,k}^{\mathrm{d}\pm} = \delta_{j+1,k}(1-\delta_{j,N}) - \delta_{j,k+1}(1-\delta_{k,N}) \mp \mathrm{i}\,\delta_{j,1}\delta_{k,N} \pm \mathrm{i}\,\delta_{j,N}\delta_{k,1}, \tag{14}$$

and $*$ denotes complex conjugation. The quadratic form (10) can be diagonalised to

$$\tilde{H} = \sum_{k=0}^{N-1} \Lambda_k \eta_k^\dagger \eta_k + e\,\mathbb{I}_N \tag{15}$$

by means of a Bogoliubov-Valatin transformation. Here, $\eta_k^\dagger$ and η_k are new fermionic creation and annihilation operators, e is a constant, and the squared fermion energies Λ_k^2 are given by the eigenvalues of the $2N \times 2N$ matrix

$$A = \begin{pmatrix} D & E \\ -E^* & -D^* \end{pmatrix}^2 = \begin{pmatrix} D^2 - EE^* & (D-D^*)E \\ -(D-D^*)E^* & (D^*)^2 - EE^* \end{pmatrix}, \tag{16}$$

see [16] for details. The matrix A has the property $CAC = A^*$, where C is the $2N \times 2N$ matrix with elements

$$C_{j,k} = \delta_{j+N,k} + \delta_{j,k+N}. \tag{17}$$

An eigenvector Φ of A corresponds to a proper Bogoliubov-Valatin transformation if it satisfies $C\phi = \phi^*$. As was shown in [16], the spectrum of A is doubly degenerate, and one can always choose the eigenvectors such that they obey the conjugation condition.

In this approach, we effectively doubled the system, which is the reason why each fermion energy occurs twice. We only need to consider "half" the eigenvalues of A, thus removing this trivial degeneracy. Furthermore, because we can change the sign of the fermion energies Λ_k in (15) by a transformation that exchanges creation and annihilation operators, resulting only in a different value of the constant in (15), we may choose all energies to be positive, and ordered, so $0 \leq \Lambda_0 \leq \Lambda_1 \leq \ldots \leq \Lambda_{k-1}$. In this case, the constant in (15) is just the corresponding ground-state energy, $e = E_0$.

For the periodic and antiperiodic mixed-sector Hamiltonians $\tilde{H}^{\pm}$ of (7), it turns out that A is in fact block-diagonal, and both blocks are identical, because all matrix elements are real. So in this case we can limit ourselves to one block immediately, and diagonalise the resulting $N \times N$ matrix. The solution of the eigenvalue equations

$$(D^2 - EE^*)^{(\pm)}\Psi_k^{(\pm)} = (\Lambda_k^{(\pm)})^2\Psi_k^{(\pm)}, \tag{18}$$

with $k = 0, 1, \ldots, N-1$, are simply given by

$$\Lambda_k^{(\pm)} = 2\sin(\tfrac{p_k^{(\pm)}}{2}), \qquad (\Psi_k^{(\pm)})_j = \exp(\mathrm{i}\, p_k^{(\pm)} j), \tag{19}$$

where the eigenvalues and the unnormalised eigenvectors are parametrised by the momenta

$$p_k^{(+)} = \frac{(2k+1)\pi}{N}, \qquad p_k^{(-)} = \frac{2k\pi}{N}. \tag{20}$$

For the duality-twisted mixed-sector Hamiltonians $\tilde{H}^{(\mathrm{d}\pm)}$ (8), the situation is more complicated, because the matrix $A^{(\mathrm{d})} := A^{(\mathrm{d}+)} = A^{(\mathrm{d}-)}$ does not have block form. Nevertheless, the bulk part of the equations, which does not involve boundary terms, is still the same and can be solved as above. The modified equations correspond to the rows 1, $N-1$, N, $N+1$, $2N-1$ and $2N$ of the matrix $A^{(\mathrm{d})}$. These yield additional conditions, so one should look for a solution involving terms $\exp(\pm\mathrm{i}\, p_k^{(\mathrm{d})} j)$ with site-dependent coefficients at the boundary. Whereas it was not possible to solve the equations in closed form for the generalised defects in [16], it is possible in this case. One arrives at the solution

$$\Lambda_k^{(\mathrm{d})} = 2|\sin(\tfrac{p_k^{(\mathrm{d})}}{2})|, \qquad p_k^{(\mathrm{d})} = \pm\frac{4k\pi}{2N-1}, \tag{21}$$

and the corresponding unnormalised eigenvectors of $A^{(\mathrm{d})}$ are

$$\begin{aligned}(\Phi_k^{(\mathrm{d})})_j = (\Phi_k^{(\mathrm{d})})^*_{j+N} = {} & \cos(\tfrac{p_k^{(\mathrm{d})}}{2})\exp(\mathrm{i}\, p_k^{(\mathrm{d})} j) \\ & + \mathrm{i}\,[\sin(\tfrac{p_k^{(\mathrm{d})}}{2}) - 1]\exp(-\mathrm{i}\, p_k^{(\mathrm{d})} j), \qquad 1 \leq j \leq N-1, \\ (\Phi_k^{(\mathrm{d})})_N = (\Phi_k^{(\mathrm{d})})^*_{2N} = {} & 1 - \sin(\tfrac{p_k^{(\mathrm{d})}}{2}). \end{aligned} \tag{22}$$

In general, positive and negative momenta in (21) give two linearly independent eigenvectors (22) for the same eigenvalue. However, there is only one vector for $k = 0$, which corresponds to the zero mode. A second, linearly independent eigenvector is

$$(\Phi_0^{(\mathrm{d})})_j = \mathrm{i}\,(\delta_{j,N} - \delta_{j,2N}), \tag{23}$$

as can easily be checked.

The fermion excitation spectra (19) and (21) determine the complete energy spectrum of the mixed-sector Hamiltonians $\tilde{H}^{(\pm)}$ (7) and $\tilde{H}^{(\mathrm{d}\pm)}$ (8), respectively, apart from the constant in (15), which corresponds to the ground-state energy of the respective Hamiltonian. This can be calculated by considering the trace of the Hamiltonian. As $\mathrm{tr}(\tilde{H}^{(\pm)}) = \mathrm{tr}(\tilde{H}^{(\mathrm{d}\pm)}) = 0$, and

$$\mathrm{tr}\left(\sum_{k=0}^{N-1} \Lambda_k \eta_k^\dagger \eta_k + E_0\,\mathbb{I}_N\right) = N\left(\frac{1}{2}\sum_{k=0}^{N-1}\Lambda_k + E_0\right), \tag{24}$$

the ground-state energies are given by

$$-E_0^{(+)} = \sum_{k=0}^{N-1} \sin(\tfrac{(k+\frac{1}{2})\pi}{N}) = \frac{1}{\sin(\frac{\pi}{2N})} = \frac{2N}{\pi} + \frac{\pi}{12N} + \mathrm{O}(N^{-3}), \tag{25}$$

$$-E_0^{(-)} = \sum_{k=0}^{N-1} \sin(\tfrac{k\pi}{N}) = \cot(\tfrac{\pi}{2N}) = \frac{2N}{\pi} - \frac{\pi}{6N} + \mathrm{O}(N^{-3}), \tag{26}$$

$$\begin{aligned} -E_0^{(\mathrm{d})} = \sum_{k=0}^{N-1} \sin(\tfrac{k\pi}{N-\frac{1}{2}}) &= \frac{1+\cos(\frac{\pi}{2N-1})}{2\sin(\frac{\pi}{2N-1})} \\ &= \frac{2(N-\frac{1}{2})}{\pi} - \frac{\pi}{24(N-\frac{1}{2})} + \mathrm{O}[(N-\tfrac{1}{2})^{-3}] \\ &= \frac{2N}{\pi} - \frac{1}{\pi} - \frac{\pi}{24N} + \mathrm{O}[N^{-2}] \end{aligned} \tag{27}$$

Comparing those with the finite-size corrections of the ground-state energy expected from conformal field theory

$$-E_0 = A_0 N + \frac{\pi c}{6N} + \mathrm{o}(N^{-1}), \tag{28}$$

we find that the ground-state energy per site in the thermodynamic limit is given by

$$A_0 = \lim_{N\to\infty}(-\frac{E_0^+}{N}) = \lim_{N\to\infty}(-\frac{E_0^-}{N}) = \lim_{N\to\infty}(-\frac{E_0^{\mathrm{d}}}{N}) = \frac{2}{\pi} \tag{29}$$

and the central charge $c = \frac{1}{2}$ for the periodic chain. The finite-size corrections for the other two cases result in "effective central charges" $\tilde{c}^- = -1$ and $\tilde{c}^{\mathrm{d}} = -1/4$, which correspond to excitations with conformal dimension $x^- = (c-\tilde{c}^-)/12 = 1/8$, the magnetisation operator, and $x^{\mathrm{d}} = (c-\tilde{c}^{\mathrm{d}})/12 = 1/16$, the "exotic" spinor operator with conformal spin $1/16$ [6]. Note that, for the latter result, the result (27) shows that it is preferable to define the scaling limit by using $N-\frac{1}{2}$ as the effective system size in (28); for the naive scaling with N, a constant surface term $A_1 = 1/\pi$ appears in (28), similar to what one finds for free or fixed boundary conditions, or in the case of defect lines [16, 17]. In that sense, the duality-twisted chain acts as a toroidal chain of $N-\frac{1}{2}$ sites rather than N sites, in accordance with the relation to the odd length spin-1/2 XXZ Heisenberg spin chain [6].

Using the appropriate scaling, the linearised low-energy spectrum becomes

$$\lim_{N\to\infty}[\frac{N}{2\pi}(\tilde{H}^+ - E_0^+\mathbb{I}_N)] = \sum_{r=0}^{\infty}[(r+\tfrac{1}{2})a_r^\dagger a_r + (r+\tfrac{1}{2})b_r^\dagger b_r] \tag{30}$$

$$\lim_{N\to\infty}[\frac{N}{2\pi}\,(\tilde{H}^{-} - E_0^{+}\mathbb{I}_N)] = \sum_{r=0}^{\infty}[r a_r^{\dagger} a_r + (r+1) b_r^{\dagger} b_r] + \frac{1}{8} \tag{31}$$

for the periodic and antiperiodic mixed-sector Hamiltonians, and simply

$$\lim_{N\to\infty}[\frac{N-\frac{1}{2}}{2\pi}\,(\tilde{H}^{\mathrm{d}\pm} - \frac{N-\frac{1}{2}}{N} E_0^{+}\mathbb{I}_N)] = \sum_{k+0}^{\infty}[r a_r^{\dagger} a_r + (r+\tfrac{1}{2}) b_r^{\dagger} b_r] + \frac{1}{16} \tag{32}$$

for the duality-twisted case, where the fermionic operators a_r and b_r are obtained from the η_k by renumbering. Taking into account the momenta, and bosonising the low-energy theory in terms of two generators L_0 and $\bar{L}_0$ of two commuting Virasoro algebras with central charge $c = \frac{1}{2}$ by means of a Sugawara construction, the first two yield the usual conformal torus partition functions $Z^{+} = (\chi_0 + \chi_{1/2})(\bar{\chi}_0 + \bar{\chi}_{1/2})$ and $Z^{-} = 2\chi_{1/16}\bar{\chi}_{1/16}$ for the Ising model, where χ_{Δ} denote the character function of the irreducible representations of the $c = \frac{1}{2}$ Virasoro algebra with highest weight Δ. Depending on the sign of the boundary term, the last corresponds to the combinations $(\chi_0 + \chi_{1/2})\bar{\chi}_{1/16}$ or $\chi_{1/16}(\bar{\chi}_0 + \bar{\chi}_{1/2})$ of characters, as derived in [6] from the relation to the XXZ Heisenberg chain with toroidal boundary conditions [8, 10, 6].

Hence, for this particular instance of conformally twisted boundary conditions, the complete spectrum is known even for finite systems, and the scaling limit can be performed explicitly. It would be interesting to know whether the more general boundary conditions introduced recently [1, 2, 3, 4, 5] can be interpreted in a similar way, and what the corresponding symmetries are that allow the definition of twisted toroidal boundary conditions.

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