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LETTER TO THE EDITOR

The 'topological' charge for the finite XX quantum chain

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Abstract. It is shown that an operator (in general non-local) commutes with the Hamiltonian describing the finite *XX* quantum chain with certain non-diagonal boundary terms. In the infinite-volume limit this operator gives the 'topological' charge.

We consider the L sites XX quantum chain with non-diagonal boundary terms given by the Hamiltonian

$$H = \frac{1}{4} \sum_{j=1}^{L-1} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \lambda \sigma_1^x + \mu [\cos(\chi) \sigma_L^x - \sin(\chi) \sigma_L^y]$$
(1)

where λ , μ and χ are parameters. Obviously the O(2) symmetry on the bulk terms is broken by the boundary terms. The question is if this finite quantum chain has any 'hidden' symmetries (hidden symmetries normally occur in the thermodynamic limit only). We will show that it does. In order to understand the problem and find the 'hidden' symmetries, it is convenient [1] to add two more sites denoted by 0 and L + 1 and consider another Hamiltonian that we denote by

$$H_{\rm f} = \frac{1}{4} \sum_{j=1}^{L-1} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \lambda \sigma_0^x \sigma_1^x + \mu [\cos(\chi) \sigma_L^x \sigma_{L+1}^x - \sin(\chi) \sigma_L^y \sigma_{L+1}^x].$$
(2)

(in [2,3] H_f was denoted by H_{long}). Note that H_f is $Z(2) \times Z(2)$ symmetric since the matrices σ_0^x and σ_{L+1}^x commute with H_f . Therefore the spectrum of H_f decomposes into four blocks $(\pm, \pm), (\pm, \mp)$ corresponding to the eigenvalues ± 1 of the σ^x matrices. The Hamiltonian H given by equation (1) corresponds to the (+, +) block. In fact, the symmetry of H_f is larger than $Z(2) \times Z(2)$, it is the finite non-Abelian group with the three generators $\sigma_0^x, \sigma_{L+1}^x$ and $U = \sigma_0^z \sigma_1^z \dots \sigma_{L+1}^z$ (which also commutes with H_f). Moreover, using the obvious relations

$$\{\sigma_0^x, U\} = \{\sigma_{L+1}^x, U\} = 0 \qquad U^2 = 1$$
(3)

one can show that if $|\mu, \nu, E\rangle$ is an eigenvector of H_f in the (μ, ν) sector, corresponding to the eigenvalue *E*, then

$$U|\mu,\nu,E\rangle = |-\mu,-\nu,E\rangle \tag{4}$$

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is also an eigenvector of H_f , in the $(-\mu, -\nu)$ sector corresponding to the same eigenvalue *E*. As a result, the whole spectrum of H_f is doubly degenerate: the spectra in the sectors (+, +) and (-, -) (respectively (+, -) and (-, +)) are identical. Since the degeneracy includes the

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ground state, the symmetry is spontaneously broken. The Hamiltonian H_f can be diagonalized in terms of free fermions which does not mean that the fermionic energies or the wavefunctions are simple to derive since the secular equation is hard to solve. This problem is discussed in detail in [2]. Moreover, for our purpose one needs to find boundary terms which lead to fermionic energies of a special form (the reason is going to be explained shortly), therefore from our collection of boundary terms where we could find solutions of the secular equation, we will consider only two kinds of boundary conditions:

$$\lambda = \mu = \frac{1}{\sqrt{8}} \tag{5}$$

$$\lambda = \mu = \frac{1}{4} \qquad \chi = 0. \tag{6}$$

We have to consider the cases L odd and even separately. The reason is the following: for L odd the ground state of H_f is in the (+, +) sector in which we are interested. For L even the ground state is in the (+, -) sector. Since we are more interested in the spectra where the ground state is, we will confine ourselves to the L odd case (as opposed to the case of diagonal boundary terms where the ground state appears in chains with an even number of sites [4]). One can repeat the whole procedure described below for L even. For both cases (5) and (6) one finds a zero-fermionic mode which explains in a different way why each level of H_f is doubly degenerate. We now specialize to the boundary condition (5). The energy gaps are given [2] by the fermionic energies (the zero mode not included)

$$\Lambda_n^{\pm} = \sin\left(\frac{2n+1}{L+1}\frac{\pi}{2} \pm \frac{\chi}{L+1}\right) \qquad 0 \leqslant n \leqslant (L-1)/2.$$
⁽⁷⁾

It is convenient to consider the operator

$$T_{\rm f} = \frac{1}{2} \sum_{n=0}^{(L-1)/2} (N_n^+ - N_n^-).$$
(8)

where N_n^{\pm} are fermionic number operators ($N_n^{\pm} = 0, 1$) corresponding to the energies given by equation (7). The eigenvalues of T_f denoted by *m* are obviously given by integer or half-integer numbers. Obviously this allows a Z(2) grading. It turns out [2] that in the (+, +) sector *m* takes integer values (an even number of fermions) whereas in the (+, -) sector it takes half-integer values (an odd number of fermions). We define the partition function corresponding to the eigenvalue *m* of T_f , for a chain with *L* sites

$$Z_m(L) = \operatorname{tr} z^{\frac{L}{\pi} \left[\sum_{n=0}^{(L-1)/2} (\Lambda_n^+ N_n^+ + \Lambda_n^- N_n^-) \right]}$$
(9)

with the constraint

$$\frac{1}{2}\sum_{n=0}^{(L-1)/2} (N_n^+ - N_n^-) = m$$
(10)

and consider the sectors (+, +) and (+, -) only. In the thermodynamic limit one obtains

$$Z_m = \lim_{L \to \infty} Z_m(L) = z^{2(m+\chi/(2\pi))^2 - \chi^2/(2\pi^2)} \prod_{n=1}^{\infty} (1-z^n)^{-1}$$
(11)

which is what one would expect if T_f corresponds to the 'topological' charge. If we consider the (+, +) sector (which as mentioned corresponds to the original Hamiltonian given by equation (1)) and sum over *m* integers the partition functions given by equation (11), one obtains the known partition function for a compactified bosonic field (with the correct radius) and von Neumann boundary conditions at both ends [3, 5, 6]. We would like to remind

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the reader that the 'topological' charge coincides with magnetic charge in the Coulomb gas problem or to the vorticity index in the Gauss model (see the classical papers [7,8] or [9] for a review on the subject). It is remarkable that we have been able to identify on the finite lattice the magnetic charge operator in the case of non-diagonal boundary conditions (for periodic boundary conditions we do not know if it exists). As is well known, for the electric charge (which is dual [7] to the magnetic charge) the corresponding operator coincides with the *z*component of the total spin of the quantum chain (1) which commutes with the finite chain Hamiltonian for periodic or diagonal boundary conditions.

The whole algebraic structure of the problem, in the thermodynamic limit, can be read-off from the expressions (7):

$$\lim_{L \to \infty} \left(\frac{L}{\pi} \Lambda_n^{\pm}\right) = n + 1/2 \pm \chi/\pi \tag{12}$$

if we keep in mind that the sum of two integer numbers is an integer number. One could pursue this issue further and make contact with the sine-Gordon model with a boundary at the free-fermion point where much work has been performed [10–12]. In this paper we are, however, interested in the properties of the finite chain given by equation (1) and therefore want to obtain the 'topological' charge T for this chain. In order to do so, we have to write T_f given by equation (8) in the basis where H_f is written (see equation (2)) and project on the (+, +) sector. This is a lengthy calculation where we have used the results of [2]. One obtains

$$T = \frac{-1}{4L+4} \sum_{\substack{k,j=1\\k\neq r \text{ odd}}}^{L} \left\{ \left[f(j-k)\cos\left(\chi\frac{k-j}{L+1}\right) - (-1)^{k}f(k+j)\cos\left(\chi\frac{k+j}{L+1}\right) \right] \right. \\ \left. \times \sigma_{k}^{y}\sigma_{k+1}^{z} \dots \sigma_{j-1}^{z}\sigma_{j}^{x} - \left[f(j-k)\cos\left(\chi\frac{k-j}{L+1}\right) + (-1)^{k}f(k+j)\cos\left(\chi\frac{k+j}{L+1}\right) \right] \right. \\ \left. \times \sigma_{k}^{x}\sigma_{k+1}^{z} \dots \sigma_{j-1}^{z}\sigma_{j}^{y} + \left[f(j-k)\sin\left(\chi\frac{k-j}{L+1}\right) + (-1)^{k}f(k+j)\sin\left(\chi\frac{k+j}{L+1}\right) \right] \right] \\ \left. \times \sigma_{k}^{y}\sigma_{k+1}^{z} \dots \sigma_{j-1}^{z}\sigma_{j}^{y} + \left[f(j-k)\sin\left(\chi\frac{k-j}{L+1}\right) - (-1)^{k}f(k+j)\sin\left(\chi\frac{k+j}{L+1}\right) \right] \right] \\ \left. \times \sigma_{k}^{x}\sigma_{k+1}^{z} \dots \sigma_{j-1}^{z}\sigma_{j}^{x} \right\} \\ \left. + \frac{1}{\sqrt{8}(L+1)}\sum_{j=1\atop j \text{ odd}}^{L} \left\{ f(j)\cos\left(\chi\frac{j}{L+1}\right)\sigma_{1}^{z} \dots \sigma_{j-1}^{z}\sigma_{j}^{y} + f(j)\sin\left(\chi\frac{j}{L+1}\right)\sigma_{1}^{z} \dots \sigma_{j-1}^{z}\sigma_{j}^{x} - f(j+L+1)\cos\left(\chi\frac{j}{L+1}\right)\sigma_{j}^{y} \\ \left. \times \sigma_{j+1}^{z} \dots \sigma_{L}^{z} - f(j+L+1)\sin\left(\chi\frac{j}{L+1}\right)\sigma_{j}^{x}\sigma_{j+1}^{z} \dots \sigma_{L}^{z} \right\}$$
(13)

where

$$f(x) = 1/\sin\left(\frac{x\pi}{2L+2}\right).$$
(14)

T is a pseudoscalar for $\chi = 0$ when H is parity invariant. One can also check that

$$[T,H] = 0 \tag{15}$$

only for L odd and not for L even. Expression (13) is 'horrible', what is important is that it exists. Let us stress that we were able to identify T_f and therefore T only because the fermionic energies had the form (7). We have not found [2] any other boundary conditions where we know the spectrum of the finite chain and where the partition functions have the form given by equation (11) with χ different to zero (only in this case we can write T_f as in equation (8)). We would have liked to have more examples in order to make sure that the boundary condition (5) is not a special case and that only for this case one can find the 'topological' charge. There is, however, one case (given by the boundary condition (6)) where although the spectrum of the finite quantum chain H is twice degenerate (nothing to do with a zero mode but with the fact that in the continuum it gives the partition function (11) with $\chi = 0$):

$$\Lambda_n^+ = \Lambda_n^- = \sin\left(\frac{2n+1}{L+2}\frac{\pi}{2}\right) \qquad 0 \leqslant n \leqslant (L-1)/2 \tag{16}$$

we were able to identify the 'topological' charge. We performed the task using a trick. We took $\lambda = \mu = 1/4$ and a small value for χ in equation (2), diagonalized H_f numerically and identified Λ_n^{\pm} and the creation and annihilation operators corresponding to these energy levels. This allowed us to guess T_f for $\chi = 0$ where the spectrum of H_f is known. We found

$$T_{\rm f} = \frac{1}{8} \sum_{j=1}^{L-1} [(1+(-1)^j)\sigma_j^x \sigma_{j+1}^y - (1-(-1)^j)\sigma_j^y \sigma_{j+1}^x] + \frac{1}{4}(\sigma_0^x \sigma_1^y - \sigma_L^y \sigma_{L+1}^x)$$
(17)

and

$$T = \frac{1}{8} \sum_{j=1}^{L-1} [(1 + (-1)^j)\sigma_j^x \sigma_{j+1}^y - (1 - (-1)^j)\sigma_j^y \sigma_{j+1}^x] + \frac{1}{4}(\sigma_1^y - \sigma_L^y).$$
(18)

Note that expressions (17) and (18) are local ones. One can look at T and consider it as a quantum chain (keep in mind that it only commutes with H for L odd). This quantum chain has amusing properties. If we disregard the boundary terms, it is trivial to diagonalize it and one obtains

$$\frac{1}{2} \left(\sum_{k=1}^{L-1} N_k \right) - \frac{L-1}{4} \tag{19}$$

here N_k are fermionic number operators. If one takes into account the boundary terms, in order to diagonalize it, one has to use T_f given by equation (17) and project in order to find the spectrum of T (the way we did in order to find the spectrum of H from the spectrum of H_f). For L odd the spectrum is the known one (integer values) since T is the 'topological' charge. For L even, the spectrum is complicated.

One can ask what we have learned from our exercise. The fact that the quantum chain (1) has many conservation laws (the total number of fermions is just one example) should not be a surprise since its spectrum is related to the one of H_f which is a free system. We think that the fact that we have been able to identify the 'topological' charge which is related to the magnetic charge in the Coulomb gas description or to vortices on a finite lattice is interesting and that this identification can probably be performed not only for the XX chain, but for the XXZ chain too. How to perform this generalization is by no means clear to us.

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