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Valence bond ground states in quantum antiferromagnets and quadratic algebras

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Abstract. The wavefunctions corresponding to the zero-energy eigenvalue of a one-dimensional quantum chain Hamiltonian can be written in a simple way using quadratic algebras. Hamiltonians describing stochastic processes have stationary states given by such wavefunctions and various quadratic algebras have been found and applied to several diffusion processes. We show that similar methods can also be applied for equilibrium processes. As an example, for a class of q-deformed O(N) symmetric antiferromagnetic quantum chains, we give the zero-energy wavefunctions for periodic boundary conditions corresponding to momenta zero and π. We also consider free and various non-diagonal boundary conditions and give the corresponding wavefunctions. All correlation lengths are derived.

1. Introduction

Quadratic algebras and their representations have been extensively used recently in order to study the probability distributions of steady states of one-dimensional stochastic processes with open boundaries or on a ring [1,2]. The basic idea is that if the Hamiltonian of a quantum chain, which gives the time evolution of the system, has eigenvalue zero, the ket wavefunctions which are related to the steady state probability distributions have a simple expression in terms of a certain quadratic algebra determined by the bulk rates. This algebra has representations fixed by the boundary conditions; the corresponding matrices act in an auxiliary vector space. All correlation functions can be computed from these ket wavefunctions. The aim of this paper is to 'import' these techniques to equilibrium statistical physics and stress the limitations and differences. For stochastic processes the lowest eigenvalue of the Hamiltonian which gives the time evolution of the system is zero. This is not the case for most of the Hamiltonians which are interesting in equilibrium problems. Therefore the possible applications of the algebraic approach to ground states is bound to be more limited. Another difference is that, in equilibrium and periodic boundary conditions, the ground state can have non-zero momentum (is not translationally invariant). This cannot be the case for stochastic processes since the components of the ground-state ket vector have to be positive numbers (they are probabilities). Another difference appears when we want to calculate correlation functions which are expressed in terms of vacuum expectation values (implying the bra and ket vacua). As we shall see the expressions of the correlation functions are very similar in the two cases. Actually the quadratic algebra approach has implicitly already been used in equilibrium problems, where it is known as the matrix product approach [3–6]. The matrices used are in fact representations of certain

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algebras. We hope to convince the reader that the algebraic approach is not only more aesthetic but more powerful, since it makes contact with known results obtained in mathematics. Finally, we would like to mention that matrix product approach has been used as an alternative to the density matrix renormalization group method [7, 8]. How the methods presented in this paper can be applied to this problem is an open question. The application of quadratic algebras to zero-energy states is presented in section 2. Much of the content of this section is already known. What is new is how to handle zone boundary states which have momentum π. In section 3 we give an application. The idea is simple: in the study of quantum groups, in order to find the non-commutative manifold in which they act, Reshetikhin *et al* [9] have introduced projector operators out of which one can build quantum chains having the quantum algebra as symmetry. Moreover, one obtains for free a quadratic algebra (the manifold of the quantum group) which can be used to write the zero-energy eigenfunctions of quantum chains built using the projector operators. These chains are not exactly integrable since there is no associated R matrix satisfying the Yang–Baxter equation [10]. We have considered, as an example, the $O(N)$ case for which we obtain an N-state Hamiltonian. The quadratic algebra turns out to be the q-deformed Clifford algebra. In the special case $N = 3$ and $q = 1$ one recovers the model with valence bond ground state (VBS) of Affleck *et al* [3]. (The q-deformed case can be found in [6, 11].) The $N = 4$ case is discussed in appendix A: it is a special case of the extended Hubbard model [12]. The Hamiltonians we consider can be mapped into quantum spin ladder models [13] and find applications in this context. We are going to show that, for periodic boundary conditions and an even number of sites, we find a unique zero-momentum ground state. For N even, we also find one zone boundary state. For free boundary conditions, we find 2^{N-1} ground states. This degeneracy can be lifted by adding boundary fields. In section 4 we show how to choose the boundary conditions in order to obtain a unique vacuum. The boundary terms break the symmetry of the quantum chain. The calculation of all the correlation lengths (for any N) is presented in section 5. It is shown that for large N the correlation lengths diverge. In appendix B we show how to compute the correlation function for some parity violating operators, appearing in the case where N is even. This problem is interesting in the case of periodic boundary conditions when the ground state is twice degenerate even for a finite number of sites. The conclusions can be found in section 6.

2. Zero-energy states and quadratic algebras

The application of quadratic algebras to the zero-energy ket wavefunctions for diffusion–reaction processes is well known [1, 2, 14], in this section we shall make a trivial extension to equilibrium processes and show how to compute correlation functions. We consider a most general one-dimensional quantum chain with N states, L sites and nearest-neighbour two-body interactions. The Hamiltonian is

$$H = \sum_{k=1}^{L-1} H_k + \mathcal{L} + \mathcal{R}. \tag{1}$$

The bulk terms ($k = 1, \ldots, L-1$) and the left and right boundary terms are

$$H_k = \sum_{\alpha,\beta,\gamma,\delta=1}^{N} \Gamma_{\gamma\delta}^{\alpha\beta} E_k^{\gamma\alpha} E_{k+1}^{\delta\beta} \tag{2}$$

$$\mathcal{L} = \sum_{\alpha,\beta=1}^{N} L_\beta^\alpha E_1^{\beta\alpha} \qquad \mathcal{R} = \sum_{\alpha,\beta=1}^{N} R_\beta^\alpha E_L^{\beta\alpha}. \tag{3}$$

Here $E_k^{\alpha\beta}$ are a basis for $N \times N$ matrices on the kth site:

$$(E^{\alpha\beta})_{\gamma\delta} = \delta_{\alpha\gamma}\delta_{\beta\delta} \qquad (\alpha, \beta, \gamma, \delta = 1, \ldots, N). \tag{4}$$

We shall assume that H has at least one eigenstate of energy zero

$$H|0\rangle = 0 \qquad \langle 0|H = 0. \tag{5}$$

Our aim is to describe the bra $\langle 0|$ and ket $|0\rangle$ states in a simple way. In order to do that, we consider two associative algebras defined by the bulk interaction:

$$\sum_{\alpha,\beta=1}^{N} \Gamma_{\gamma\delta}^{\alpha\beta} x_\alpha x_\beta = x_\gamma X_\delta - X_\gamma x_\delta \tag{6}$$

$$\sum_{\gamma,\delta=1}^{N} \Gamma_{\gamma\delta}^{\alpha\beta} y_\gamma y_\delta = y_\alpha Y_\beta - Y_\alpha y_\beta. \tag{7}$$

If the bulk part of the Hamiltonian is not symmetric, the two algebras are different. Each algebra has $2N$ generators x_α, X_α and y_α, Y_α, $(\alpha = 1, \ldots, N)$, respectively. We define two Fock-like representations of the two algebras:

$$\langle V_K|\left(X_\alpha - \sum_{\beta=1}^{N} L_\alpha^\beta x_\beta\right) = 0 \qquad \left(X_\alpha + \sum_{\beta=1}^{N} R_\alpha^\beta x_\beta\right)|W_K\rangle = 0 \tag{8}$$

$$\langle V_B|\left(Y_\beta - \sum_{\alpha=1}^{N} L_\alpha^\beta y_\alpha\right) = 0 \qquad \left(Y_\beta + \sum_{\alpha=1}^{N} R_\alpha^\beta y_\alpha\right)|W_B\rangle = 0. \tag{9}$$

Here $\langle V_K|$, $|W_K\rangle$, $\langle V_B|$ and $|W_B\rangle$ are the bra and ket reference states defined by the equations (8) and (9) in auxiliary spaces. We make now the connexion between the two algebras and the zero-energy eigenstates of the Hamiltonian. The basis in the ket vector space in which the Hamiltonian acts is

$$u_{\alpha_1} u_{\alpha_2}, \ldots, u_{\alpha_L} \qquad (\alpha_k = 1, 2, \ldots, N) \tag{10}$$

the N-dimensional vector u_{α_k} is in the kth site and has the component α_k equal to one and the others zero:

$$(u_{\alpha_k})_\beta = \delta_{\alpha_k,\beta} \qquad (\beta = 1, 2, \ldots, N). \tag{11}$$

We denote the basis in the bra vector space in which the Hamiltonian acts by

$$u_{\alpha_1}^{\mathrm{T}} u_{\alpha_2}^{\mathrm{T}}, \ldots, u_{\alpha_L}^{\mathrm{T}}. \tag{12}$$

The scalar product is obviously

$$\langle u_{\alpha_k}^{\mathrm{T}} u_{\beta_k}\rangle = \delta_{\alpha_k,\beta_k}. \tag{13}$$

One can prove [15] that the unnormalized bra and ket vacua can be written using the two quadratic algebras:

$$|0\rangle = \sum_{\alpha_1,\ldots,\alpha_L=1}^{N} \langle V_K|x_{\alpha_1}, \ldots, x_{\alpha_L}|W_K\rangle u_{\alpha_1}, \ldots, u_{\alpha_L} \tag{14}$$

$$\langle 0| = \sum_{\alpha_1,\ldots,\alpha_L=1}^{N} \langle V_B|y_{\alpha_1}, \ldots, y_{\alpha_L}|W_B\rangle u_{\alpha_1}^{\mathrm{T}}, \ldots, u_{\alpha_L}^{\mathrm{T}}. \tag{15}$$

Notice that the generators X_α and Y_α do not appear in the expressions of the wavefunctions. One can also show that the quadratic algebras exist, and that one can find representations satisfying the conditions (8) and (9). Moreover, one can show that all the zero-energy wavefunctions can

be obtained in this way [15]. In the case of periodic boundary conditions, and translationally invariant zero-energy eigenfunctions, one can use the expressions (14) and (15), making the substitution

$$\langle V_K|\cdots|W_K\rangle \to \mathrm{Tr}(\cdots) \qquad \langle V_B|\cdots|W_B\rangle \to \mathrm{Tr}(\cdots) \tag{16}$$

provided that the algebra has a trace operation.

As opposed to the case of the Hamiltonian with open boundaries, for periodic boundary conditions, it is not clear in which cases one obtains in this way all the zero-energy eigenfunctions. A simple counter-example was given in [16], in which it is shown that there are zero-energy eigenfunctions which cannot be obtained using the algebraic method given by equation (16). On the other hand, examples are known [17] where indeed all the eigenfunctions are obtained.

Ground-state wavefunctions can correspond to zone boundary states (momentum π). One can show that if the algebra (6) has the Str operation with the properties

$$\begin{aligned} \mathrm{Str}(x_{\alpha_1}x_{\alpha_2},\ldots,x_{\alpha_L}) &= -\mathrm{Str}(x_{\alpha_L}x_{\alpha_1}x_{\alpha_2},\ldots,x_{\alpha_{L-1}}) \\ \mathrm{Str}(X_{\alpha_1}x_{\alpha_2},\ldots,x_{\alpha_L}) &= -\mathrm{Str}(x_{\alpha_L}X_{\alpha_1}x_{\alpha_2},\ldots,x_{\alpha_{L-1}}) \end{aligned} \tag{17}$$

then the ket vector

$$|0\rangle = \sum_{\alpha_1,\ldots,\alpha_L=1}^{L} \mathrm{Str}(x_{\alpha_1},\ldots,x_{\alpha_L})u_{\alpha_1},\ldots,u_{\alpha_L} \tag{18}$$

satisfies equation (5) and is obviously a zone boundary state. Similar expressions can be used for the algebra (7) and the bra eigenvector. The Str (called supertrace) operation is taken from the theory of superalgebras and it implies that the x_α and X_α are odd generators in this algebra. In particular if in the algebra (6) one takes X_α c-numbers (this is often done for diffusion processes [2]), the algebra cannot have the Str operation. In section 3 we shall show in examples how the Str operation works. As for translationally invariant ground states it is not known whether all of the zone boundary states can be obtained using equation (18).

Before showing how to compute correlation functions, let us see what are the consequences for the quadratic algebras of the existence of a symmetry of the Hamiltonian. Let us assume that the operator

$$A = \sum_{k=1}^{L}\sum_{\mu,\nu=1}^{N} A_{\mu\nu}E_k^{\mu\nu} \tag{19}$$

commutes with the bulk part of the Hamiltonian, i.e.

$$\left[A, \sum_{k=1}^{L-1} H_k\right] = 0. \tag{20}$$

Simple arithmetics gives the relations

$$\begin{aligned} &\sum_{\alpha,\beta,\mu=1}^{N} \Gamma_{\gamma\delta}^{\alpha\beta}[(A_{\alpha\mu}x_\mu)x_\beta + x_\alpha(A_{\beta\mu}x_\mu)] \\ &\qquad = \sum_{\mu=1}^{N}[(A_{\gamma\mu}x_\mu)X_\delta + x_\gamma(A_{\delta\mu}X_\mu) - (A_{\gamma\mu}X_\mu)x_\delta - X_\gamma(A_{\delta\mu}x_\mu)]. \end{aligned} \tag{21}$$

The above relations are obtained by using (6) and multiplying each two-body term arising from (20) by $\sum_{l,m,n,o=1}^{N} E_k^{l,n}E_{k+1}^{m,o}x_l x_m$. The relation (21) gives a set of simplified algebraic relations among the generators of the algebra and, at the same time, shows that the generators

are tensor operators. (A relation similar to (21) can be obtained for the generators y_α and Y_α.) As an example, let us choose $A_{11} = 1$ and all the other matrix elements zero in (19). Using (21) one obtains

$$\sum_{\alpha=1}^{N}(\Gamma_{\gamma\delta}^{1\alpha}x_1x_\alpha + \Gamma_{\gamma\delta}^{\alpha 1}x_\alpha x_1) = \delta_{\gamma,1}(x_1X_\delta - X_1x_\delta) + \delta_{\delta 1}(x_\gamma X_1 - X_\gamma x_1). \tag{22}$$

Similar relations can be obtained in the case of quantum algebra symmetries when the operator A does not have the simple expression (19). We now show how to compute a two-point function. This calculation is interesting when the ground-state energy is zero. Consider two local operators P_r and Q_s on the r and s sites. They act on the basis (10) as follows:

$$P_r u_{\alpha_r} = \sum_{\beta_r=1}^{N} P_{\beta_r,\alpha_r} u_{\beta_r} \qquad Q_s u_{\alpha_s} = \sum_{\beta_s=1}^{N} Q_{\beta_s,\alpha_s} u_{\beta_s}. \tag{23}$$

We want to compute the expression

$$G_{r,s} = \frac{\langle 0|P_r Q_s|0\rangle}{Z} \tag{24}$$

where $\langle 0|$ and $|0\rangle$ are given by equations (14) and (15) and Z is a normalization factor originating from the fact that (14) and (15) give unnormalized wavefunctions. It is useful to define the following quantities (all related to the auxiliary space):

$$C = \sum_{\alpha=1}^{N} x_\alpha \otimes y_\alpha \tag{25}$$

$$P = \sum_{\alpha,\beta=1}^{N} P_{\alpha\beta}x_\beta \otimes y_\alpha \qquad Q = \sum_{\alpha,\beta=1}^{N} Q_{\alpha,\beta}x_\beta \otimes y_\alpha \tag{26}$$

and

$$\langle V_B| \otimes \langle V_K| = \langle V| \qquad |W\rangle = |W_K\rangle \otimes |W_B\rangle. \tag{27}$$

Using equations (25)–(27), the two-point function (22) has the following simple expression:

$$G_{r,s} = \frac{1}{Z}\langle V|C^{r-1}PC^{s-r-1}QC^{L-s}|W\rangle \tag{28}$$

where

$$Z = \langle V|C^L|W\rangle. \tag{29}$$

Notice that C plays the role of a space evolution operator in the auxiliary space but the analogy with a quantum mechanical problem cannot be pushed further since $\langle V|$ and $|W\rangle$ are not eigenfunctions of C. Nevertheless one can see that the spectrum of C gives all the correlation lengths. For periodic boundary conditions, we have to make the following substitution:

$$\begin{aligned}\langle V|\cdots|W\rangle &\to \mathrm{Tr}(\cdots)\\ \langle V|\cdots|W\rangle &\to \mathrm{Str}(\cdots)\end{aligned} \tag{30}$$

for translationally invariant states, or for zone boundary states, in equations (28) and (29). Let us observe that the expressions (25)–(29) are similar to the ones obtained for stochastic processes [1, 2]. The difference is that instead of dealing with only one algebra (given by equation (6)), one has the tensor product of two algebras. If the algebra (7) has a one-dimensional representation (this is always the case for diffusion processes with exclusion for example [1]), the correlation functions computed using the ket vector only or the bra and ket vector (vacuum expectation values) coincide. Expressions such as (25)–(29) have been

used in a different context in the matrix product approach to the density matrix renormalization group method [7]. In this case the x_α are matrices obtained using the variational method and not using quadratic algebras defined by the Hamiltonian using equation (6). Besides they have to satisfy the condition

$$\sum_{\alpha=1}^{N} x_\alpha x_\alpha^+ = 1. \tag{31}$$

As we shall see in the next section, this condition is not necessarily fulfilled in our applications.

3. q-deformed O(N) symmetric, N-state quantum chains

The quantum chains describing stochastic processes are given by non-Hermitian Hamiltonians, which always have zero as lowest eigenvalue. The quadratic algebra always exists [15] and the problem is to find representations of the algebra. In equilibrium problems one is interested in Hermitian Hamiltonians, which in general do not have zero as the lowest eigenvalue and therefore one has to find Hamiltonians which have this property. In order to illustrate the method, in this paper we have chosen an easy way: using known results in the theory of quantum groups. In this way we obtain not only Hermitian quantum chains which have zero for the ground-state energy but also quadratic algebras with known representations.

3.1. The bulk Hamiltonian

Reading the paper of Reshetikhin *et al* [9] one can notice that there are several expressions of the form (6) with the X_{α_s} equal to zero. We shall choose the one where $\Gamma^{\alpha\beta}_{\gamma\delta}$ are projector operators of rank $N(N+1)/2-1$ for the q-deformed $B(n)$ series ($N=2n+1$) and $D(n)$ series ($N=2n$) [19]. The x_α are the generators of the non-commutative algebra of the manifold where the quantum groups act. Similar expressions for the $Sp(n)$ and $Osp(m/n)$ algebras and superalgebras can also be obtained [18]. In this paper, we confine ourselves to the q-deformed O(N) case. As we shall show we shall use these projectors in order to write Hamiltonians for quantum chains. The projector operators have the following expressions:

$$\begin{aligned} P_k^{(+)} = \sum_{\alpha,\beta,\gamma,\delta=1}^{N} \Gamma^{\alpha\beta}_{\gamma\delta} E_k^{\gamma\alpha} E_{k+1}^{\delta\beta} = \frac{1}{q+q^{-1}} \Bigg[& q \sum_{\alpha\neq\alpha'} E_k^{\alpha\alpha} E_{k+1}^{\alpha\alpha} + (q-q^{-1}) \sum_{\alpha>\beta} E_k^{\beta\beta} E_{k+1}^{\alpha\alpha} \\ & + \delta_{N,2n+1} E_k^{\frac{N+1}{2}\frac{N+1}{2}} E_{k+1}^{\frac{N+1}{2}\frac{N+1}{2}} + q^{-1} \sum_{\alpha,\beta=1}^{N} E_k^{\alpha\alpha} E_{k+1}^{\beta\beta} + \sum_{\alpha\neq\beta,\beta'} E_k^{\beta\alpha} E_{k+1}^{\alpha\beta} \\ & + q^{-1} \sum_{\alpha\neq\alpha'} E_k^{\alpha\alpha'} E_{k+1}^{\alpha'\alpha} - \frac{q^{-\frac{N}{2}}}{[\frac{N}{2}]_q} \sum_{\alpha,\beta=1}^{N} E_k^{\alpha'\beta} E_{k+1}^{\alpha\beta'} q^{\rho_\alpha-\rho_\beta} \\ & - (q-q^{-1}) \sum_{\alpha>\beta} E_k^{\alpha'\beta} E_{k+1}^{\alpha\beta'} q^{\rho_\alpha-\rho_\beta} \Bigg] \end{aligned} \tag{32}$$

where q is a deformation parameter (taken as real in this paper) and we use the notation

$$[n]_q = \frac{q^n - q^{-n}}{q-q^{-1}} \qquad \text{and} \qquad \alpha' = N+1-\alpha \qquad (\alpha = 1, \ldots, N). \tag{33}$$

In equation (32) we also denote

$$(\rho_1, \ldots, \rho_N) = (n-\tfrac{1}{2}, n-\tfrac{3}{2}, \ldots, \tfrac{1}{2}, 0, -\tfrac{1}{2}, \ldots, -n+\tfrac{1}{2}) \tag{34}$$

for $N = 2n + 1$, and

$$(\rho_1, \ldots, \rho_N) = (n-1, n-2, \ldots, 1, 0, 0, -1, \ldots, -n+1) \tag{35}$$

for $= 2n$. By definition we have

$$(P_k^{(+)})^2 = P_k^{(+)}. \tag{36}$$

Since the matrix $\Gamma^{\alpha\beta}_{\gamma\delta}$ in (32) is symmetric, i.e. $\Gamma^{\alpha\beta}_{\gamma\delta} = \Gamma^{\gamma\delta}_{\alpha\beta}$, the two algebras associated with the projector (32)

$$\sum_{\alpha,\beta=1}^{N} \Gamma^{\alpha\beta}_{\gamma\delta} x_\alpha x_\beta = 0 \qquad \text{and} \qquad \sum_{\alpha,\beta=1}^{N} \Gamma^{\alpha\beta}_{\gamma\delta} y_\alpha y_\beta = 0 \tag{37}$$

are identical and therefore we give only one of them. It is convenient to denote (for obvious reasons) for $N = 2n$

$$\begin{array}{lll} x_1 = a_n & x_2 = a_{n-1}, \ldots & x_n = a_1 \\ x_{n+1} = a_1^+ & x_{n+2} = a_2^+, \ldots & x_{2n} = a_n^+ \end{array} \tag{38}$$

and for $N = 2n + 1$

$$\begin{array}{llll} x_1 = a_n & x_2 = a_{n-1}, \ldots & x_n = a_1 & x_{n+1} = \dfrac{1}{\sqrt{s+s^{-1}}}\Sigma \\ x_{n+2} = a_1^+, \ldots & x_{2n+1} = a_n^+ & & \end{array} \tag{39}$$

where $s = \sqrt{q}$. Inserting (38) and (39) in (37) we obtain the following relations for the $2n$ q-deformed fermionic creation and annihilation operators a_α, a_α^+ and the 'γ^5'-type generator Σ:

$$\begin{array}{ll} qa_\beta a_\alpha + a_\alpha a_\beta = 0 & (\beta > \alpha) \\ qa_\beta a_\alpha^+ + a_\alpha^+ a_\beta = 0 & (\beta > \alpha) \\ \Sigma a_\alpha + qa_\alpha \Sigma = 0 \qquad \Sigma^+ = \Sigma & \\ a_\alpha a_\alpha^+ + a_\alpha^+ a_\alpha = qa_{\alpha+1}a_{\alpha+1}^+ + q^{-1}a_{\alpha+1}^+ a_{\alpha+1} & (1 \leqslant \alpha \leqslant n-1) \\ qa_1 a_1^+ + q^{-1}a_1^+ a_1 = \Sigma^2. & \end{array} \tag{40}$$

Using equation (40), one can check that the x_αs defined by equations (38) and (39) verify the relations (37) in which we have used the equation (32) for the definition of $\Gamma^{\alpha\beta}_{\gamma\delta}$ [9].

The algebra (40) has a central element:

$$\zeta = a_n a_n^+ + a_n^+ a_n \tag{41}$$

and an obvious representation is

$$\begin{array}{ll} a_k = 1 \otimes 1 \otimes \cdots \otimes a \otimes s^{\sigma^z}\sigma^z \otimes s^{\sigma^z}\sigma^z \otimes \cdots \otimes s^{\sigma^z}\sigma^z & (k = 1, \ldots, n) \\ \Sigma = s^{\sigma^z}\sigma^z \otimes s^{\sigma^s}\sigma^z \otimes \cdots \otimes s^{\sigma^z}\sigma^z & \end{array} \tag{42}$$

with

$$a = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad a^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{43}$$

In the first line of (42) the operator a is in the kth position, and the operator $s^{\sigma^z}\sigma^z$ appears in the positions $k+1, \ldots, n$. The fact that the algebra has finite-dimensional representations makes all calculations much simpler (see sections 5 and 6) as compared with the cases when the algebra has infinite-dimensional representations. Notice also that for $q \neq 1$ the generators x_α do not satisfy the relation (31). We make now the connexion between the projectors (32) and the quantum chain (1). Since the lowest eigenvalue E of a projector operator is zero, we can choose in (1)

$$H_k = P_k^{(+)}. \tag{44}$$

Notice that H_k is Hermitian and therefore since as mentioned its lowest eigenvalue is zero, H for periodic or free boundary conditions has also zero as its lowest eigenvalue. The problem of other boundary conditions will be discussed in section 4.

3.2. Ground states for periodic and free boundary conditions

We start with periodic boundary conditions. We first consider zero-momentum states. Using equation (14) (together with the substitution given by (16) as well as the representation (42) we obtain, for all N, one single ket vector of energy zero for L even and none for L odd. This result is confirmed by the spectra obtained from the numerical diagonalization of several Hamiltonians (various L and N). This check was necessary since as mentioned in section 2 there is no theorem which assures us that there are no zero-energy eigenfunctions which are not obtained using the algebraic procedure. We now look for zone boundary states and therefore look for a definition of the Str operation such that the relations (17) and (18) are satisfied. We consider the matrix J defined by

$$J = \sigma^z \otimes \sigma^z \otimes \cdots \otimes \sigma^z. \tag{45}$$

A vector

$$|v\rangle = |v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_n\rangle \tag{46}$$

is called even (odd) if it is an eigenvector of J corresponding to the eigenvalue $+1$ (-1). A matrix is called even if it takes an even (odd) vector into an even (odd) vector. A matrix is called odd if it takes an even (odd) vector into an odd (even) vector. For example, the matrices a_k in equation (42) are odd but the matrix Σ is even. Consider now the matrix

$$A = A_1 \otimes A_2 \otimes \cdots \otimes A_n. \tag{47}$$

We define

$$\mathrm{Str}(M) = \mathrm{Tr}(JM). \tag{48}$$

It is easy to check that if A and B are odd matrices, then

$$\mathrm{Str}(AB) = -\mathrm{Str}(BA). \tag{49}$$

If one of the two matrices is even and the other one is odd

$$\mathrm{Str}(AB) = 0. \tag{50}$$

If the two matrices A and B are even

$$\mathrm{Str}(AB) = \mathrm{Str}(BA). \tag{51}$$

From this properties we learn that in order to satisfy the relations (17) (the relations in the second line of (18) are automatically satisfied since $X_\alpha = 0$), the x_αs have to be all odd generators. This excludes the case of $N = 2n + 1$ because of the appearance of the sigma generator, which is even. For L odd and $N = 2n$ all the supertraces are zero and again we cannot obtain a boundary state which is physically correct. For N and L even we expect therefore a unique zone boundary state. This is what is also seen in numerical diagonalizations for all L except for $q = 1$ and small values of L where something subtle happens. We illustrate the phenomenon taking $N = 4$. Using equations (42), (45) and (48) we obtain

$$\mathrm{Str}(a_2^+ a_2) = 0 \qquad \mathrm{Str}(a_1^+ a_1) = q - q^{-1} \tag{52}$$

which would imply that for $q = 1$ and $L = 2$ there are no zone boundary states. Actually there are two of them; they can be obtained by taking, instead of J given by equation (45), two alternative expressions:

$$1 \otimes \sigma^z \qquad \text{or} \qquad \sigma^z \otimes 1. \tag{53}$$

These expressions cannot be used however for monomials with more than two generators (the property (17) is no longer valid). In the spectra for periodic boundary conditions as seen in numerical diagonalizations, there are no zero-energy states besides those mentioned above. The existence for N even of a degenerate ground state, one of positive parity (momentum zero, obtained with the help of the Tr operation) that we denote by $|0,+\rangle$ and one of negative parity (momentum π, obtained with the help of the Str operation) that we denote by $|0,-\rangle$, allows for the existence of correlation functions of operators which break parity. For example one of the operators P or Q in equation (25) can break parity. In appendix B we show how to compute the correlation functions for this case (one considers matrix elements $\langle 0,-|\cdots|0,+\rangle$ for example). A somewhat similar problem occurs in spontaneously dimerized spin ladders [20]. We would like to stress that in our case the degeneracy of the vacuum occurs even for a finite number of sites.

We now consider free boundary conditions. An inspection of equation (8) shows that it brings no constraints, therefore instead of equation (14) we have

$$|0\rangle = \sum_{\alpha_1,\ldots,\alpha_L=1}^{N} x_{\alpha_1},\ldots,x_{\alpha_L}u_{\alpha_1},\ldots,u_{\alpha_L} \tag{54}$$

where the various independent monomials (words) in the algebra are regarded as a basis in a vector space. Each component of $|0\rangle$ in this basis gives a zero-energy eigenfunction. Therefore for both L even and odd we obtain 2^{N-1} states. This result was obtained by counting the independent words. For small values of L, the degeneracy can be smaller since higher-degree monomials might not yet have appeared. For example for $N=4$ and $L=2$ the degeneracy is seven instead of eight but for $L=3$ one obtains already eight.

4. Boundary conditions compatible with the quadratic algebras

The boundary matrices $\mathcal{L}$ and $\mathcal{R}$ (we shall choose them as Hermitian) have not only to be compatible with the quadratic algebra (see below), but have also to leave the value zero as the lowest eigenvalue. This property is guaranteed if the lowest eigenvalues E_L and E_R are also zero. This follows from the relation

$$E_H \geqslant E_L + (L-1)E + E_R \tag{55}$$

where E_H and E are the lowest eigenvalues of H and H_k.

Since, for the q-deformed O(N) symmetric quantum chains defined in the last section, the algebras (6) and (7) with X_α and Y_β equal to zero are identical, we have to find the matrices $\mathcal{L}$ and $\mathcal{R}$ as well as the vacua of the auxiliary spaces such that the following relations (obtained from equations (8), (9)) are satisfied:

$$\sum_{\beta=1}^{N} R_\alpha^\beta x_\beta |W_K\rangle = 0 \qquad \sum_{\alpha=1}^{N} R_\alpha^\beta x_\alpha |W_B\rangle = 0 \tag{56}$$

$$\sum_{\beta=1}^{N} L_\beta^\alpha \langle V_K| x_\beta = 0 \qquad \sum_{\alpha=1}^{N} L_\beta^\alpha \langle V_B| x_\alpha = 0. \tag{57}$$

We have taken the same representation for the two sets of Clifford generators x_α and y_α. We now show that the solutions of equations (57) can be obtained from those of (56). We take the transpose of the two equations (57):

$$\sum_{\beta=1}^{N} L_\beta^\alpha x_\beta^{\mathrm{T}} |V_K^{\mathrm{T}}\rangle = 0 \qquad \sum_{\alpha=1}^{N} L_\beta^\alpha x_\alpha^{\mathrm{T}} |V_B^{\mathrm{T}}\rangle = 0 \tag{58}$$

and since, from equations (38), (39), we have $x_\alpha^{\mathrm{T}} = x_{\alpha'} = x_{N+1-\alpha}$, we can rewrite the equations (58) as follows:

$$\sum_{\beta=1}^{N} L_{\beta'}^{\alpha} x_\beta |V_K^{\mathrm{T}}\rangle = 0 \qquad \sum_{\alpha=1}^{N} L_{\beta}^{\alpha'} x_\alpha |V_B^{\mathrm{T}}\rangle = 0. \tag{59}$$

We can compare now the equations (56) and (59) and deduce that for any solution R_α^β of (56) (there are many of them) one obtains a solution for L_α^β:

$$L_\beta^\alpha = R_{\beta'}^{\alpha'}. \tag{60}$$

One can use of course one solution of equations (56) for R_α^β and another solution to obtain L_α^β using equation (60). We are looking for solutions of a factorized form:

$$R_\beta^\alpha = r e_\alpha f_\beta \tag{61}$$

where r, e_α and f_β are functions which depend on the specific value of N. It is convenient to choose the following basis in the auxiliary vector spaces in which x_α and y_α (replaced formally by x_α) act (see equations (42), (43) and (56)):

$$|W_K\rangle = \left(\prod_{i=1}^{L} \frac{1}{\sqrt{1+\eta_i^2}}\right) \begin{pmatrix} \eta_1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} \eta_2 \\ 1 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} \eta_n \\ 1 \end{pmatrix} \tag{62}$$

$$|W_B\rangle = \left(\prod_{i=1}^{L} \frac{1}{\sqrt{1+\tilde{\eta}_i^2}}\right) \begin{pmatrix} \tilde{\eta}_1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} \tilde{\eta}_2 \\ 1 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} \tilde{\eta}_n \\ 1 \end{pmatrix}. \tag{63}$$

We are going to consider separately the cases $N = 2, 3, \ldots, 6$ in order to illustrate the structure of the solutions. As we shall show for $N = 2$, the values of η_1 and $\tilde{\eta}_1$ are fixed and, besides a common factor, the matrix elements of $\mathcal{R}$ contain no parameters. For $N = 3$ and 4, the parameters η_1, η_2 and $\tilde{\eta}_1$, $\tilde{\eta}_2$ respectively are free and $\mathcal{R}$ is given by the parameters of the wavefunctions (62), (63) and a common factor. For $N = 5$ and 6, a new phenomenon appears. The wavefunction (62) is given by the free parameters η_1, η_2, η_3, and the wavefunction (63) is specified by the corresponding parameters $\tilde{\eta}_1$, $\tilde{\eta}_2$, $\tilde{\eta}_3$. $\mathcal{R}$ depends now not only on the parameters of the wavefunctions but on supplementary free parameters. This implies that different boundary conditions are compatible with the same wavefunctions (14), (15). We now consider the boundary conditions for some values of N.

$N = 2$. Since this is a very simple (and trivial) case, we discuss it in detail. From equations (32) and (44) we obtain

$$H_k = \tfrac{1}{2}(\sigma_k^z \sigma_{k+1}^z + 1). \tag{64}$$

This implies that for free boundary conditions the ground state is twice degenerate, with antiferromagnetic ordering. This degeneracy is a consequence of the existence of two independent words in the O(2) algebra: $x_1x_2, \ldots, x_1x_2$ and $x_2x_1, \ldots, x_2x_1$. Demanding that $\mathcal{R}$ is diagonalizable, equations (56) have two solutions:

$$\mathcal{R} = rA \qquad |W_K\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |W_B\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{65}$$

and

$$\mathcal{R} = rB \qquad |W_K\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad |W_B\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{66}$$

where

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{67}$$

and $r > 0$.

We consider separately the two cases.

(a) $\mathcal{R} = rA$, $\mathcal{L} = lA$ with $r, l > 0$. For lattice size L even, we obtain no zero-energy eigenstate. The matrix elements (14), (15) vanish. For L odd, one obtains a unique zero-energy ground state.

(b) $\mathcal{R} = rA, \mathcal{L} = lB$ For L even, one obtains an unique zero-energy ground state and none for L odd.

$N = 3$. The solutions are

$$\begin{array}{lll} f_1 = s\eta_1 & f_2 = -\sqrt{s + s^{-1}} & f_3 = -(s\eta_1)^{-1} \\ e_1 = s\tilde{\eta}_1 & e_2 = -\sqrt{s + s^{-1}} & e_3 = (s\tilde{\eta}_1)^{-1} \end{array} \tag{68}$$

and the eigenvalues of $\mathcal{R}$ are zero twice and

$$r\left[1 + \frac{1}{s + s^{-1}}(s^2\eta_1\tilde{\eta}_1 + (s^2\eta_1\tilde{\eta}_1)^{-1})\right]: \tag{69}$$

this relation imposes $r > 0$. Since we want $\mathcal{R}$ symmetric, we take (see equation (61)) $\eta_1 = \tilde{\eta}_1$ and therefore

$$e_\alpha = f_\alpha (\alpha = 1, 2, \ldots, N). \tag{70}$$

$N = 4$. One obtains

$$f_1 = s\eta_2 \qquad f_2 = -\eta_1 \qquad f_3 = -\eta_1^{-1} \qquad f_4 = -(s\eta_2)^{-1}. \tag{71}$$

The matrix $\mathcal{R}$ has three eigenvalues zero and one equal to

$$r[(s\eta_2)^2 + \eta_1^2 + \eta_1^{-2} + (s\eta_2)^{-2}]. \tag{72}$$

Notice that for $N = 3$ and 4, the parameters of the vacua and r determine the $\mathcal{R}$ matrix. This is bound to change for larger values of N.

$N = 5$. The solution is

$$\begin{array}{lll} f_1 = \eta_2 s\left(1 + a\dfrac{s - s^{-1}}{s + s^{-1}}\right) & f_2 = -\eta_1(1 - a) & f_3 = -\dfrac{2a}{\sqrt{s + s^{-1}}} \\ f_4 = -\eta_1^{-1}(a + 1) & f_5 = -\eta_2^{-1}s^{-1}\left(1 + a\dfrac{s - s^{-1}}{s + s^{-1}}\right) & \end{array} \tag{73}$$

where a is an additional free parameter. $\mathcal{R}$ has now four eigenvalues zero and one equal to $r\sum_{i=1}^{5} f_i^2$.

$N = 6$. One obtains

$$\begin{array}{lll} f_1 = \eta_3 s\left(a + \dfrac{s - s^{-1}}{2}\right) & f_2 = -\eta_2\left(a - \dfrac{s + s^{-1}}{2}\right) & f_3 = -\eta_1 \\ f_4 = -\eta_1^{-1} & f_5 = -\eta_2^{-1}\left(a + \dfrac{s + s^{-1}}{2}\right) & f_6 = -s^{-1}\eta_3^{-1}\left(a + \dfrac{s - s^{-1}}{2}\right) \end{array} \tag{74}$$

with a arbitrary. $\mathcal{R}$ has now five eigenvalues zero and one equal to $r\sum_{i=1}^{6} f_i^2$.

Notice that for $N = 5$ and 6 the fs depend not only on η_1, η_2 and η_3 but also on the supplementary parameter a. This implies that the same wavefunction can be used for different boundary matrices. We also notice that taking r positive ensures that the lowest eigenvalue remains zero. One can obtain $\mathcal{R}$ matrices with only non-vanishing elements on the diagonal (as in equation (67)), taking one of the η_i equal to zero or infinity. This remains valid for any N. For larger values of N the number of free parameters increases and it is certainly not our purpose to give here the general solution. We would like to stress that for $N > 2$ the boundary conditions can break all the symmetries of the Hamiltonian.

5. Diagonalization of the C matrix and calculation of the correlation lengths of the q-deformed O(N) quantum chain

It is necessary to have a new look at the expression (28) of the two-point correlation function. In the last section we have shown how to obtain the bra and ket vacua ($\langle V|$ and $|W\rangle$, respectively) in the auxiliary spaces. In order to proceed further, one has to find the similarity transformation S which diagonalizes the matrix C:

$$C = SC_DS^{-1}. \tag{75}$$

The matrix C is given by equation (25). In this equation the x_α and y_α are the generators of the two identical algebras (see (38)–(40)) having the representation (42), (43). We shall consider separately the cases where N is even or odd.

(a) $N = 2n$

It is convenient to write C as a four-state Hamiltonian with n sites in the auxiliary space:

$$C^{(N)} = E_1F_2F_3, \ldots, F_n + E_2F_3F_4, \ldots, F_n + \cdots + E_n \tag{76}$$

where the matrices E_i and F_i act on the ith site and have the expression

$$E = a \otimes a = \begin{array}{c} \begin{matrix} {\scriptstyle (1,1)} & {\scriptstyle (1,2)} & {\scriptstyle (2,1)} & {\scriptstyle (2,2)} \end{matrix} \\ \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \end{array} \tag{77}$$

$$F = s^{\sigma^z}\sigma^z \otimes s^{\sigma^z}\sigma^z = \begin{array}{c} \begin{matrix} {\scriptstyle (1,1)} & {\scriptstyle (1,2)} & {\scriptstyle (2,1)} & {\scriptstyle (2,2)} \end{matrix} \\ \begin{pmatrix} q & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & q^{-1} \end{pmatrix} \end{array} \tag{78}$$

where

$$a = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{79}$$

The basis vectors in the tensor products (77), (78) correspond to the two-dimensional representations used in (42), (43). In this basis the vacuum $|W\rangle$ in the auxiliary space has the expression

$$|W\rangle = V^{(1)} \otimes V^{(2)} \otimes \cdots \otimes V^{(n)} \tag{80}$$

where

$$V = \frac{1}{\sqrt{(1+\eta^2)(1+\tilde{\eta}^2)}} \begin{pmatrix} \eta \\ 1 \end{pmatrix} \otimes \begin{pmatrix} \tilde{\eta} \\ 1 \end{pmatrix}. \tag{81}$$

Notice the recurrence relation:

$$C^{(N+2)} = C^{(N)} F_{n+1} + E_{n+1} \tag{82}$$

that we are going to use later on. If $q = 1$, the diagonalization of C is trivial since E and F commute. Using the similarity transformation

$$U = \frac{\sqrt{2}}{2} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \tag{83}$$

we have

$$E_D = UEU^{-1} = \tfrac{1}{2}(\sigma^z \otimes 1 + 1 \otimes \sigma^z) \qquad F_D = U^{-1}FU = \sigma^z \otimes \sigma^z. \tag{84}$$

It is convenient to write C_D as a one-dimensional two-state spin chain with $2n$ sites:

$$\begin{aligned} C_D^{(N)} = \tfrac{1}{2}[&(\sigma_1^z + \sigma_2^z)(\sigma_3^z\sigma_4^z)\cdots(\sigma_{2n-1}^z\sigma_{2n}^z) \\ &+(\sigma_3^z + \sigma_4^z)(\sigma_5^z\sigma_6^z)\cdots(\sigma_{2n-1}^z\sigma_{2n}^z) + \cdots + (\sigma_{2n-1}^z + \sigma_{2n}^z)]. \end{aligned} \tag{85}$$

In order to simplify the expression (85), it is useful to look at C as a function defined on the Abelian group $Z_2 \otimes Z_2 \otimes \cdots \otimes Z_2 = (Z_2)^{\otimes 2n}$. In order to do so, we write

$$\sigma_k^z = (-1)^{\epsilon_k} \qquad (\epsilon_k = 0, 1). \tag{86}$$

Using this notation, instead of equation (85) we obtain

$$\begin{aligned} C_D^{(N)} = \tfrac{1}{2}[&((-1)^{\epsilon_1} + (-1)^{\epsilon_2})((-1)^{\epsilon_3}(-1)^{\epsilon_4})\cdots((-1)^{\epsilon_{2n-1}}(-1)^{\epsilon_{2n}}) \\ &+((-1)^{\epsilon_3} + (-1)^{\epsilon_4})((-1)^{\epsilon_5}(-1)^{\epsilon_6})\cdots((-1)^{\epsilon_{2n-1}}(-1)^{\epsilon_{2n}}) \\ &+\cdots + ((-1)^{\epsilon_{2n-1}} + (-1)^{\epsilon_{2n}})]. \end{aligned} \tag{87}$$

We perform now the change of variables:

$$\begin{aligned} \omega_1 &= \epsilon_1 + (\epsilon_3 + \epsilon_4) + \cdots + (\epsilon_{2n-1} + \epsilon_{2n}) \\ \omega_2 &= \epsilon_2 + (\epsilon_3 + \epsilon_4) + \cdots + (\epsilon_{2n-1} + \epsilon_{2n}) \\ \omega_3 &= \epsilon_3 + (\epsilon_5 + \epsilon_6) + \cdots + (\epsilon_{2n-1} + \epsilon_{2n}) \\ \omega_4 &= \epsilon_4 + (\epsilon_5 + \epsilon_6) + \cdots + (\epsilon_{2n-1} + \epsilon_{2n}) \\ &\vdots \\ w_{2n-1} &= \epsilon_{2n-1} \\ w_{2n} &= \epsilon_{2n}. \end{aligned} \tag{88}$$

Notice the identity

$$(-1)^{\sum_{i=1}^N \omega_i} = (-1)^{\sum_{i=1}^N \epsilon_i} \tag{89}$$

that we are going to use shortly. With the change of variables (88), instead of the expression (87), we obtain

$$C_D^{(N)} = \tfrac{1}{2}\sum_{i=1}^{N}(-1)^{\omega_i} = \tfrac{1}{2}\sum_{i=1}^{N}\tau_i^z = S_{(N)}^z. \tag{90}$$

From equation (90) it turns out that the spectrum of $C^{(N)}$ for $N = 2n$ is the same as that of the z-component of the total spin S^z for $2n$ spins $\frac{1}{2}$. Therefore the eigenvalues are $n - m$ ($m = 0, 1, \ldots, N$) with a degeneracy given by the binomial coefficient C_N^{N-m}.

We now consider the case $q \neq 1$. We are going to use the recurrence relation (76). We first make a change of basis (see equations (77), (78)) in the four-state chain with n sites:

$$(1, 1) \to 1 \qquad (2, 2) \to 2 \qquad (1, 2) \to 3 \qquad (2, 1) \to 4 \tag{91}$$

and denote by $u_i^{(k)}$, the basis vector on the kth site having the ith ($i = 1, 2, 3, 4$) component equal to one and the others zero. In this basis E and F have the expressions

$$E = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad F = \begin{pmatrix} q & 0 & 0 & 0 \\ 0 & q^{-1} & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{92}$$

In the same basis, for $N = 2$, one has

$$C^{(2)} = E_1 \tag{93}$$

and the eigenvalues (eigenfunctions) are

$$1, \left[\frac{u_1^{(1)} + u_2^{(2)}}{\sqrt{2}}\right] \qquad -1, \left[\frac{u_1^{(1)} - u_2^{(2)}}{\sqrt{2}}\right] \qquad 0, [u_3^{(1)}] \qquad 0, [u_4^{(1)}]. \tag{94}$$

Assume that $\Psi_\Lambda^{(N)}$ written in the basis

$$u_{\alpha_1}^{(1)} u_{\alpha_2}^{(2)}, \ldots, u_{\alpha_n}^{(n)} \qquad (\alpha_i = 1, 2, 3, 4)$$

is an eigenfunction of $C^{(N)}$ corresponding to the eigenvalue Λ. We now consider the four wavefunctions

$$\Psi_\Lambda^{(N)} u_i^{(n+1)} \qquad (i = 1, 2, 3, 4) \tag{95}$$

and act with $C^{(N+2)}$ on them using the relation (82). We obtain

$$\begin{aligned} C_\Lambda^{(N+2)} \Psi_\Lambda^{(N)} u_1^{(n+1)} &= \Lambda q \Psi_\Lambda^{(N)} u_1^{(n+1)} + \Psi_\Lambda^{(N)} u_2^{(n+1)} \\ C_\Lambda^{(N+2)} \Psi_\Lambda^{(N)} u_2^{(n+1)} &= \Lambda q^{-1} \Psi_\Lambda^{(N)} u_2^{(n+1)} + \Psi_\Lambda^{(N)} u_1^{(n+1)} \\ C_\Lambda^{(N+2)} \Psi_\Lambda^{(N)} u_3^{(n+1)} &= -\Lambda \Psi_\Lambda^{(N)} u_3^{(n+1)} \\ C_\Lambda^{(N+2)} \Psi_\Lambda^{(N)} u_4^{(n+1)} &= -\Lambda \Psi_\Lambda^{(N)} u_4^{(n+1)}. \end{aligned} \tag{96}$$

Two of the wavefunctions (95) for $i = 3$ and 4 are therefore eigenfunctions of $C^{(N+2)}$ corresponding to the same eigenvalue $-\Lambda$. One obtains also the two other eigenvalues:

$$\Omega^{\pm} = \tfrac{1}{2}\left[\Lambda(q + q^{-1}) \pm \sqrt{\Lambda^2 (q - q^{-1})^2 + 4}\right]. \tag{97}$$

Notice that if $\Lambda = [m]_q$, then $\Omega^{\pm} = [m \pm 1]_q$, where we have used the notation (33). The eigenfunctions corresponding to the eigenvalues $\Omega^{\pm}$ are

$$\Psi_\Lambda^{(N)} (u_1^{(n+1)} + (\Omega^{(\pm)} - q\Lambda) u_2^{(n+1)}). \tag{98}$$

Using the eigenvalues and eigenfunctions (94) for $N = 2$ and the recurrence relations (96)–(98) one can obtain all the eigenvalues and eigenfunctions of $C^{(N)}$ for any even N. The eigenvalues are

$$[n - m]_q \qquad (m = 0, \ldots, N) \tag{99}$$

with a degeneracy

$$C_N^{N-m}. \tag{100}$$

For $q = 1$ one recovers the spectrum given by $S_{(N)}^z$ (see equation (90)). Notice that the similarity transformations used here are even matrices (see section 3.2), therefore the supertrace operation defined by equation (48) remains valid.

(b) $N = 2n + 1$

We start again with $q = 1$ and from the definition of $C^{(2n+1)}$ we have

$$C^{(2n+1)} = C^{(2n)} + \tfrac{1}{2}\prod_{k=1}^{2n}\sigma_k^z. \tag{101}$$

Using the equations (86) and (89), (90), we obtain the diagonal form of $C^{(2n+1)}$:

$$C_D^{(2n+1)} = S_{(2n)}^z + \tfrac{1}{2}(-1)^{n+S_{(2n)}^z} \tag{102}$$

which obviously has the spectrum

$$\frac{N}{2} - 2m \qquad (m = 0, 1, 2, \ldots, n) \tag{103}$$

with a degeneracy

$$C_N^{2m}. \tag{104}$$

We now consider the case $q \neq 1$. Instead of (101) one has

$$C^{(2n+1)} = C^{(2n)} + \frac{1}{s + s^{-1}} F_1 F_2, \ldots, F_n. \tag{105}$$

The recurrence relation (82) remains valid as well as (96)–(98). As opposed to $N = 2n$, where we use the recurrence relations starting with $C^{(2)}$, for $N = 2n + 1$ we start with $C^{(3)}$. In the basis $u_i^{(1)}$ $(i = 1, 2, 3, 4)$, the matrix $C^{(3)}$ is

$$C^{(3)} = \frac{1}{s + s^{-1}} \begin{pmatrix} s^2 & (s + s^{-1}) & 0 & 0 \\ (s + s^{-1}) & s^{-2} & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{106}$$

having obviously the following eigenvalues (eigenfunctions):

$$\left[\frac{3}{2}\right]_q, \left[\frac{1}{\sqrt{1+q}}(\sqrt{q}u_1^{(1)} + u_2^{(1)})\right] \qquad -\left[\frac{1}{2}\right]_q, \left[\frac{1}{\sqrt{1+q}}(u_1^{(1)} - \sqrt{q}u_2^{(1)})\right]$$
$$-\left[\frac{1}{2}\right]_q, [u_3^{(1)}] \qquad -\left[\frac{1}{2}\right]_q [u_4^{(1)}]. \tag{107}$$

The spectrum of $C^{(2n+1)}$ is therefore

$$\left[\frac{N}{2} - 2m\right]_q \qquad (m = 0, 1, \ldots, n) \tag{108}$$

with a degeneracy

$$C_{2n+1}^{2m}. \tag{109}$$

From the spectra of the matrix C, which plays the role of a transfer matrix (see equation (28)), one can derive the mass spectra (the inverse of the correlation lengths) using equations (99) and (108). For $N = 2n$ we have

$$M_m = \ln \frac{[\frac{N}{2}]_q}{[\frac{N}{2} - m]_q} \qquad (m = 1, \ldots, n - 2) \tag{110}$$

and for $N = 2n + 1$ we obtain

$$M_m = \ln \frac{[\frac{N}{2}]_q}{[\frac{N}{2} - 2m]_q} \qquad (m = 1, \ldots, n). \tag{111}$$

Therefore the system is always massive. It is interesting to note that in the large-N limit, for $q = 1$, one obtains (see equations (110), (111))

$$\begin{aligned} &\lim_{N\to\infty} \frac{N}{2} M_m = m \qquad (N = 2n) \\ &\lim_{N\to\infty} \frac{N}{2} M_m = 2m \qquad (N = 2n+1). \end{aligned} \tag{112}$$

This implies that in the limit $N \to \infty$, all correlation lengths diverge. Looking at the expressions (112) and keeping in mind that in conformal invariant theories one has similar expressions with N substituted by L (N of O(N) replacing L, the size of the system, of the conformal invariant quantum chain), we would expect some similarity between the two physics. The analogy, however, is not so simple since the degeneracy of the level m also diverges (see equations (100) and (109)). An explicit calculation of the correlation functions in the large-N limit, which we did not perform, will clarify the issue.

It is interesting to notice that for O(3), spin S, $(2S + 1)$-state quantum chain VBS gives, for the the smallest mass M_1, the following large-S behaviour [4]:

$$\lim_{S\to\infty} \frac{S}{2} M_1 = 1. \tag{113}$$

Comparing the equations (112) with (113) we learn that, in the asymptotic cases, the largest correlation length is given essentially by the number of states of the chain.

6. Conclusions

We have considered q-deformed O(N) symmetric, N-state quantum chains defined by Hamiltonians given by equations (1), (32) and (44). The symmetry is unbroken for free boundary conditions. For $q \neq 1$ the quantum group symmetry is broken for periodic boundary conditions. For $q = 1$, no symmetry might remain because of boundary terms which can be chosen as described in section 4. Using algebraic methods, the ground-state wavefunctions for these quantum chains are known exactly for periodic, free and non-diagonal boundary conditions; they all correspond to energy zero. The wavefunctions are obtained using q-deformed Clifford algebras. These generalize the construction of Affleck *et al* [3]. Using the trace and supertrace operations in an auxiliary space, for N even and periodic boundary conditions, one obtains two ground states, one for momentum zero and one for momentum π. This implies that, even for a finite number of sites and periodic boundary conditions, the ground state is degenerate. For N odd one obtains only translationally invariant ground states. For free boundary conditions the degeneracy of the ground state is 2^{N-1}. This degeneracy is lifted by boundary terms. We have shown how to compute correlation functions and have derived all the correlation lengths. They are finite and diverge only for $q = 1$ and $L \to \infty$. What is the physical relevance of our results? For $N = 4$ we have shown in appendix A how the chain can be mapped into the extended Hubbard model [12]. For all values of N one can map our quantum chains for obvious reasons into various ladder models [13], writing the on-rung interaction as a two-site interaction. Whether what one obtains is physically interesting remains to be seen. On the other hand the wavefunctions we obtain can be used as trial ground states for more realistic models [3]. Can the procedure described here be extended to other quantum chains? The answer is yes. One can consider q-deformed $Sp(N)$ symmetric chains. In this case instead of the Clifford algebra one obtains [18] the q-deformed Heisenberg algebra as a tool to compute the wavefunctions. One can go even one step further and take quantum chains with the superalgebra $Osp(M/N)$ as symmetry. In this case [18] the algebra one uses to construct the wavefunctions is a combination of the Clifford and Heisenberg algebras. These extensions

are straightforward. Again, it is an open question whether these extensions are interesting from a physical point of view. Last but not least, very simple quadratic algebras were discussed above; whether more interesting ones (with X_α and Y_α in equations (6) and (7) unequal to zero) find use in equilibrium problems remains to be seen. They do in non-equilibrium problems.

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Appendix A. Fermionic formulation of the O(4) quantum chain

In this appendix we shall present explicitly the Hamiltonian that corresponds to the $N = 4$ case. From (32) and (34) the Hamiltonian is

$$H = \sum_k H_k \tag{A.1}$$

$$\begin{aligned}
H_k = P_k^{(+)} &= \sum_{\alpha,\beta,\gamma,\delta=1}^{4} \Gamma_{\gamma\delta}^{\alpha\beta} E_k^{\gamma\alpha} E_{k+1}^{\delta\beta} \\
&= \frac{1}{q+q^{-1}}\{(q+q^{-1})[E_k^{11}E_{k+1}^{11} + E_k^{22}E_{k+1}^{22} + E_k^{33}E_{k+1}^{33} + E_k^{44}E_{k+1}^{44}] \\
&\quad +q[E_k^{11}E_{k+1}^{22} + E_k^{11}E_{k+1}^{33} + E_k^{22}E_{k+1}^{44} + E_k^{33}E_{k+1}^{44}] \\
&\quad +q^{-1}[E_k^{33}E_{k+1}^{11} + E_k^{44}E_{k+1}^{33} + E_k^{44}E_{k+1}^{22} + E_k^{22}E_{k+1}^{11}] \\
&\quad +[E_k^{21}E_{k+1}^{12} + E_k^{12}E_{k+1}^{21} + E_k^{31}E_{k+1}^{13} + E_k^{13}E_{k+1}^{31} \\
&\quad +E_k^{42}E_{k+1}^{24} + E_k^{24}E_{k+1}^{42} + E_k^{43}E_{k+1}^{34} + E_k^{34}E_{k+1}^{43}] \\
&\quad +\alpha_3[E_k^{22}E_{k+1}^{33} + E_k^{33}E_{k+1}^{22} + E_k^{14}E_{k+1}^{41} + E_k^{23}E_{k+1}^{32} + E_k^{32}E_{k+1}^{23} + E_k^{41}E_{k+1}^{14}] \\
&\quad +\alpha_1 E_k^{11}E_{k+1}^{44} + \alpha_5 E_k^{44}E_{k+1}^{11} + \alpha_2[E_k^{31}E_{k+1}^{24} + E_k^{21}E_{k+1}^{34} + E_k^{12}E_{k+1}^{43} + E_k^{13}E_{k+1}^{42}] \\
&\quad +\alpha_4[E_k^{42}E_{k+1}^{13} + E_k^{43}E_{k+1}^{12} + E_k^{34}E_{k+1}^{21} + E_k^{24}E_{k+1}^{31}]\}
\end{aligned} \tag{A.2}$$

where

$$\begin{aligned}
&\alpha_1 = \frac{q^3}{1+q^2} \qquad \alpha_2 = -\frac{q^2}{1+q^2} \qquad \alpha_3 = \frac{q}{1+q^2} \\
&\alpha_4 = -\frac{1}{1+q^2} \qquad \alpha_5 = \frac{q^{-1}}{1+q^2}.
\end{aligned} \tag{A.3}$$

It is also interesting to rewrite (A.2) in terms of spin-$\frac{1}{2}$ creation and annihilation fermion operators on the lattice. This is done by making the following correspondence between the basis $|\alpha\rangle_j$, $\alpha = 1, 2, 3, 4$, in (A.2), at each lattice point j, and the Fock representation:

$$\begin{aligned}
&|1\rangle_j \leftrightarrow |0\rangle_j = |\cdot\ \cdot\rangle_j \qquad |2\rangle_j \leftrightarrow c_{j,+}^{+}|0>_j = |\uparrow\ \cdot\rangle_j \\
&|3\rangle_j \leftrightarrow c_{j,-}^{+}|0\rangle_j = |\cdot\ \downarrow\rangle_j \qquad |4\rangle_j \leftrightarrow c_{j,+}^{+}c_{j,-}^{+}|0\rangle_j = |\uparrow\downarrow\rangle_j.
\end{aligned} \tag{A.4}$$

Using this fermionic basis the Hamiltonian density (A.2) is given by

$$H_k = \frac{1}{q+q^{-1}}\left\{ \sum_{\sigma=+,-} (c_{k,\sigma}^{+}c_{k+1,\sigma} + \text{h.c.})(1 + t_{\sigma 1}n_{k,-\sigma} + t_{\sigma 2}n_{k+1,-\sigma} + t'_\sigma n_{k,-\sigma}n_{k+1,-\sigma}) \right.$$

$$+J(\vec{S}_k \cdot \vec{S}_{k+1} - n_k n_{k+1}/4) + t_p(c^+_{k,+}c^+_{k,-}c_{k+1,+}c_{k+1,-} + \text{h.c.}) + (q+q^{-1})$$
$$-qn_k - q^{-1}n_{k+1} + U_l n_{k,+}n_{k,-} + U_r n_{k+1,+}n_{k+1,-} + \sum_{\sigma,\sigma'=+,-} V_{\sigma,\sigma'} n_{k,\sigma}n_{k+1,\sigma'}$$
$$+[V_3^{(1)} n_{k,+}n_{k+1,-}n_{k+1,+} + V_3^{(2)} n_{k,-}n_{k+1,-}n_{k+1,+} + V_3^{(3)} n_{k,-}n_{k,+}n_{k+1,+}$$
$$+V_3^{(4)} n_{k,-}n_{k,+}n_{k+1,-}] + V_4 n_{k,-}n_{k,+}n_{k+1,-}n_{k+1,+}\Big\} \tag{A.5}$$

where

$$t_{-1} = t_{+1} = -\frac{q^2+2}{q^2+1} \qquad t_{-2} = t_{+2} = -\frac{1+2q^2}{1+q^2} \qquad t'_- = t'_+ = 3$$
$$J = 2t_p = \frac{2q}{1+q^2} \qquad U_l = \frac{q^3}{1+q^2} \qquad U_r = \frac{q^{-1}}{1+q^2} \tag{A.6}$$
$$V_{++} = V_{--} = q+q^{-1} \qquad V_{+-} = V_{-+} = \frac{2q}{1+q^2}$$
$$V_3^{(1)} = V_3^{(2)} = -q^{-1} \qquad V_3^{(3)} = V_3^{(4)} = -q \qquad V_4 = q+q^{-1}.$$

In (A.5) appear the density operators $n_{k,\sigma} = c^+_{k,\sigma}c_{k,\sigma}$ and $n_k = n_{k,+} + n_{k,-}$ at the site k. The magnetic spin–spin interaction (coupling J) in (A.5) is derived from the relation

$$\sum_{\sigma\neq\sigma'} c^+_{k,\sigma}c^+_{k+1,\sigma'}c_{k,\sigma'}c_{k+1,\sigma} = 2(\vec{S}_k \cdot \vec{S}_{k+1} - n_k n_{k+1}/4) + n_{k,+}n_{k+1,-} + n_{k,-}n_{k+1,+} \tag{A.7}$$

where $\vec{S}_k = \frac{1}{2}\vec{\sigma}_k$, and $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are the spin-$\frac{1}{2}$ Pauli matrices.

The Hamiltonian (A.5) belongs to the class of extended Hubbard models considered in the recent literature [12]. Beyond the magnetic interaction (coupling J) we also have non-diagonal interactions that correspond to single-particle correlated hopping (couplings $t_{\sigma 1}, t_{\sigma 2}, t'_\sigma; \sigma = \pm$), as well as pair hopping terms (coupling $t_{\rm p}$). The static interactions are given by the diagonal terms. The couplings U_l and U_r give us the on-site Coulomb interaction, and the interactions $V_{\sigma,\sigma'}$ $(\sigma, \sigma' = \pm)$, $V_3^{(\alpha)}$, $(\alpha = 1, \ldots, 4)$ and V_4 give us the two- three- and four-body static interactions, respectively.

We should notice that the Hamiltonian (A.5) conserves separately the total number of up spins n_+ and down spins n_-. Consequently for free boundary conditions we may construct, using the the algebraic method, zero-energy eigenfunctions Ψ_{n_+,n_-}, for each sector labelled by n_+ and n_- $(n_+, n_- = 0, 1, \ldots, L)$, i.e.

$$\Psi_{n_+,n_-} = \mathcal{P}_{n_+,n_-}\left[\prod_{\otimes k=1}^{L}(x_1 + x_2 c^+_{k,+} + x_3 c^+_{k,-} + x_4 c^+_{k,+}c^+_{k,-})|0\rangle_k\right] \tag{A.8}$$

where $\mathcal{P}_{n_+,n_-}$ projects out states which do not have n_+ spins $\sigma = +$ and n_- spins $\sigma = -$ (see equation (54)).

Appendix B. Correlation functions for parity violating operators (N even)

We would like to show how to compute the correlation functions

$$\xi_{r,s} = \frac{\langle 0, -|P_r Q_s|0, +\rangle}{Z_{-,+}} \tag{B1}$$

where

$$Z_{-,+} = \langle 0, -|0, +\rangle \tag{B2}$$

which appear for N and L even and periodic boundary conditions when the vacuum is degenerate. Here

$$|0,+\rangle = \mathrm{Tr}(x_{\alpha_1},\ldots,x_{\alpha_L})u_{\alpha_1},\ldots,u_{\alpha_L} \tag{B3}$$

corresponds to the parity +, momentum zero wavefunction,

$$\langle 0,-| = \mathrm{Str}(y_{\beta_1},\ldots,y_{\beta_L})u^T_{\beta_1},\ldots,u^T_{\beta_L} = \mathrm{Tr}(Jy_{\beta_1},\ldots,y_{\beta_L})u^T_{\beta_1},\ldots,u^T_{\beta_L} \tag{B4}$$

corresponds to the parity $-$, momentum π wavefunction. The matrix J is defined in equation (45). The action of the operators P and Q is shown equation (23). For obvious reasons, one of the two operators P or Q has to break parity. It is easy to show, using the definitions given by equations (23) and (25) that we have

$$\langle 0,-|P_r Q_s|0,+\rangle = \mathrm{Tr}(DC^{r-2}PC^{s-r-1}QC^{L-s}) \tag{B5}$$

and

$$\langle 0,-|0,+\rangle = \mathrm{Tr}(DC^{L-1}) \tag{B6}$$

where

$$D = \sum_{\alpha=1}^{N} x_\alpha \otimes Jy_\alpha. \tag{B7}$$

Obviously the correlation lengths appearing for this type of correlation function are the same as for the parity conserving operators where one computes quantities such as $\langle 0,+|,\ldots,|0,+\rangle$ or $\langle 0,-|,\ldots,|0,-\rangle$.

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