PT symmetry on the lattice: the quantum group invariant XXZ spin chain

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Abstract

We investigate the PT-symmetry of the quantum group invariant XXZ chain. We show that the PT-operator commutes with the quantum group action and also discuss the transformation properties of the Bethe wavefunction. We exploit the fact that the Hamiltonian is an element of the Temperley–Lieb algebra in order to give an explicit and exact construction of an operator that ensures quasi-Hermiticity of the model. This construction relies on earlier ideas related to quantum group reduction. We then employ this result in connection with the quantum analogue of Schur–Weyl duality to introduce a dual pair of C-operators, both of which have closed algebraic expressions. These are novel, exact results connecting the research areas of integrable lattice systems and non-Hermitian Hamiltonians.

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1. Introduction

Recent years have seen growing interest in non-Hermitian Hamiltonians and their interpretation in quantum mechanics (see [1–5] and references therein). There are several motivations to study such systems. Non-Hermitian Hamiltonians appear to be physically interesting: they can arise in connection with perturbative or effective descriptions of physical phenomena. More generally, it has been suggested that Hermiticity should not be the decisive criterion in deciding whether the associated quantum mechanics system is physically sound, but rather the reality of its spectrum (see the recent reviews [6, 7] and references therein). However, in order to ensure the unitarity of the time evolution operator one is necessarily led back to the requirement of a Hermitian Hamiltonian. The way out is the introduction of a new inner

product on the Hilbert space of quantum states with respect to which the Hamilton operator becomes Hermitian.

To be concrete, let us consider a Hamiltonian H defined on a Hilbert space $\mathfrak{H}$ with inner product $\langle \cdot, \cdot \rangle : \mathfrak{H} \times \mathfrak{H} \to \mathbb{C}$. Suppose H is non-Hermitian with respect to the inner product $\langle \cdot, \cdot \rangle$, i.e.

$$H \neq H^* \tag{1}$$

with $*$ denoting the Hermitian adjoint (or complex conjugate transpose in the case of matrices). Provided there exists a *self-adjoint, invertible and positive* operator $\eta : \mathfrak{H} \to \mathfrak{H}$ such that

$$\eta H = H^* \eta, \tag{2}$$

one can introduce another, different inner product

$$\langle \cdot, \cdot \rangle_\eta : \mathfrak{H} \times \mathfrak{H} \to \mathbb{C}, \qquad \langle x, y \rangle_\eta := \langle x, \eta y \rangle \tag{3}$$

with respect to which the Hamiltonian is now Hermitian,

$$\langle x, Hy \rangle_\eta = \langle Hx, y \rangle_\eta, \qquad x, y \in \mathfrak{H}. \tag{4}$$

Since $\eta > 0$, it possesses a unique positive square root which we denote by $\eta^{\frac{1}{2}} : \mathfrak{H} \to \mathfrak{H}$. Thus, one might alternatively consider the Hamiltonian

$$\tilde{H} = \eta^{\frac{1}{2}} H \eta^{-\frac{1}{2}} \tag{5}$$

which is Hermitian with respect to the original inner product $\langle \cdot, \cdot \rangle$,

$$\tilde{H}^* = \eta^{-\frac{1}{2}} H^* \eta^{\frac{1}{2}} = \tilde{H}. \tag{6}$$

Non-Hermitian Hamiltonians which allow for the existence of such a positive map η have been named *quasi-Hermitian* in the literature, see [8, 9] and references therein. Note that while the property of quasi-Hermiticity obviously ensures the reality of the spectrum of H, the converse is not true. In fact, in this paper we will consider a non-Hermitian Hamilton operator which for special values of a coupling parameter has a real spectrum but does not allow for a positive map η satisfying (2) unless a reduction of the state space is carried out first.

It is thus desirable for practical purposes to find a simple criterion which allows one to decide whether a given non-Hermitian Hamiltonian might in fact be quasi-Hermitian. Based on a large number of examples, it has been suggested that such a criterion is PT-symmetry, namely the invariance of the Hamiltonian under a simultaneous change of parity P and time reversal T (see the review [6] and references therein). While this has proved to be an effective way of singling out many quasi-Hermitian Hamilton operators within the pool of non-Hermitian ones, PT-symmetry of the Hamiltonian alone is not mathematically sufficient to establish even the reality of the spectrum due to the fact that time reversal is an anti-linear operator [10].

Nevertheless, in this paper we also investigate a Hamiltonian which is PT-symmetric. This symmetry is in our case even distinguished in light of an underlying algebraic structure which we are going to exploit to establish its quasi-Hermiticity. Thus, our example will confirm once more the usefulness of PT-symmetry as a pre-selection tool for quasi-Hermitian Hamilton operators.

Alternative approaches to constructing η have been pursued in the literature (for references we refer the reader to the reviews [6, 7]). One is based on the explicit solution of the eigenvalue problem of the Hamiltonian and through the construction of bi-orthonormal systems. Other approaches rest on the perturbation theory and the Baker–Campbell–Hausdorff formula. Both methods have practical limitations, in particular the former suffers from the fact that one seldom has exact expressions for all the eigenfunctions. It is in this context that integrable

or exactly solvable systems play a special role as they allow one in principle to obtain exact, non-perturbative information. Previous applications of integrable systems in the context of non-Hermitian Hamiltonians include, for example, the correspondence between integrable systems and ordinary differential equations (see [11] for a recent review). One might also directly consider non-Hermitian deformations of integrable systems respecting PT-symmetry; recent examples are discussed in [12, 13].

In this paper, we shall consider a well-known integrable quantum Hamiltonian [14, 17, 18] which for certain values of a parameter q is non-Hermitian. The novel aspect here is that we introduce the concept of PT-symmetry and the so-called C-operator for a discrete lattice model. Namely, we are going to consider the quantum group invariant *XXZ* spin-chain Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^{N-1} \left\{ \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta_+ \left(\sigma_i^z \sigma_{i+1}^z - 1 \right) \right\} + \Delta_- \frac{\left(\sigma_1^z - \sigma_N^z \right)}{2}. \tag{7}$$

Here, the anisotropy parameters $\Delta_\pm$ are defined in terms of the single variable q,

$$\Delta_\pm = \frac{q \pm q^{-1}}{2}, \tag{8}$$

and $\left\{ \sigma_i^{x,y,z} \right\}$ denote the Pauli matrices acting on the ith site of the spin chain represented by the state space $\mathfrak{H} = (\mathbb{C}^2)^{\otimes N}$. We will focus on the case when the complex parameter q lies on the unit circle $\mathbb{S}^1$; this implies that H is non-Hermitian,

$$q \in \mathbb{S}^1 : \qquad H \neq H^*. \tag{9}$$

This case of q on the unit circle is of particular interest, since then the corresponding lattice model is believed to correspond in the thermodynamic limit to a conformal field theory with central charge [14, 17]

$$c = 1 - \frac{6}{(r-1)r}, \qquad q = \exp\left(\frac{i\pi}{r} \right). \tag{10}$$

When $r \in \mathbb{N}, r > 2$, i.e. q is a root of unity, the above central charge value matches that from the minimal unitary series. Besides this connection with the conformal field theory, which has fuelled ongoing interest in this particular spin-chain Hamiltonian, there are several algebras which play an important role in the eigenvalue problem of this Hamiltonian. One is its quantum group invariance, the other is its connection with the Hecke and Temperley–Lieb algebras. We will use the representation theory of these algebras to obtain explicit and exact expressions for η. To our knowledge, there are only a few, simple systems where this has been previously achieved (see the reviews [6, 7]).

Our aim is to connect the discussion of quasi-Hermitian Hamilton operators and PT-symmetry with a procedure known as *quantum group reduction at roots of unity* in the integrable lattice models community. While this latter procedure was introduced a long time ago [19], its connection with the more recent discussion of non-Hermitian Hamilton operators has not been previously investigated. Moreover, we will derive for this particular case novel expressions for η in terms of the Hecke algebra, thus giving a purely algebraic definition of the new Hilbert space structure in which (5) is Hermitian. We will also consider a special segment of the unit circle where q is not a root unity. For this case, no reduction of the state space is required.

The content of this paper is as follows. In section 2, we recall the relevant algebraic structures. We hope that this section will keep the paper self-contained and make it more accessible to a wider audience, in particular the community working on non-Hermitian Hamilton operators. In section 3, we introduce the concept of PT-symmetry on the lattice,

explaining its connection with quasi-Hermiticity. This exposition is aimed primarily at researchers in the field of integrable systems. We go on to discuss the relation of the P and T operators with the action of our two algebras. We also give the action of PT on the Bethe wavefunction. In section 4, we give a construction of η in terms of the path basis for q a root of unity (see equation (87)). In section 5, we define a C operator as $C = P\eta$ and give a simple, purely algebraic realization of it in terms of a certain braid operator associated with the Hecke algebra. We also define another operator C' that has properties that are similar to C and yet is loosely speaking 'dual' to it. In particular, C is an element of the Hecke algebra that commutes with the quantum group, while C' is an element of the quantum group that commutes with the Hecke algebra. Finally, we make some concluding comments in section 6.

2. The XXZ chain and its related algebras

As mentioned in the introduction, we will exploit several algebraic structures associated with the spin-chain Hamiltonian in order to establish its quasi-Hermiticity. In this section, we review the definition of these algebras and their relation to the Hamiltonian to keep this paper self-contained. For details concerning the definitions of the various algebras and their properties we refer the reader to e.g. [20].

2.1. The Temperley–Lieb and Hecke algebra

To make contact with the first algebra, we rewrite the spin-chain Hamiltonian (7) in terms of 'local' operators which only contain nearest-neighbour interactions,

$$H = \sum_{i=1}^{N-1} E_i, \qquad E_i = \frac{\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y}{2} + \Delta_+ \frac{\sigma_i^z \sigma_{i+1}^z - 1}{2} + \Delta_- \frac{\sigma_i^z - \sigma_{i+1}^z}{4}. \tag{11}$$

Let $V = \mathbb{C}^2$ be a two-dimensional complex vector space, then these 'local Hamiltonians' E_i provide a particular representation

$$\pi_{TL} : TL_N(q) \to \text{End } V^{\otimes N}, \qquad e_i \mapsto \pi_{TL}(e_i) := E_i \tag{12}$$

of an abstract algebra $TL_N(q)$, known as the Temperley–Lieb algebra.

Definition 2.1 (Temperley–Lieb Algebra). *The Temperley–Lieb algebra $TL_N(q)$ is obtained from $N - 1$ generators $\{e_1, e_2, \ldots, e_{N-1}\}$ satisfying the commutation relations*

$$\begin{aligned} e_i^2 &= -(q + q^{-1})e_i, & e_i e_{i\pm 1} e_i &= e_i, \\ e_i e_j &= e_j e_i, & |i - j| &> 1. \end{aligned} \tag{13}$$

In the present context, the Temperley–Lieb algebra plays the role of a spectrum generating algebra. Note that the representation defined by (11) is non-Hermitian for q on the unit circle. This is most easily seen when expressing the Temperley–Lieb generators as 4 by 4 matrices acting on the ith and $(i + 1)$th factor in the spin chain,

$$E_i = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -q^{-1} & 1 & 0 \\ 0 & 1 & -q & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_{i,i+1} \neq \bar{E}_i = E_i^*. \tag{14}$$

The irreducible representations of the Temperley–Lieb algebra will be discussed in the subsequent sections of this paper and in appendix A.

The Temperley–Lieb algebra is closely related to another algebra which can be thought of as a generalization or q-deformation of the group algebra of the symmetric group.

Definition 2.2 (Hecke algebra)**.** *The Hecke algebra $H_N(q)$ is obtained from $N-1$ generators $\{b_i\}_{i=1}^{N-1}$ obeying the defining relations,*

$$b_i b_i^{-1} = b_i^{-1} b_i = 1, \qquad b_i b_{i+1} b_i = b_{i+1} b_i b_{i+1},$$
$$b_i b_j = b_j b_i, \qquad |i-j| > 1 \tag{15}$$

and the quadratic relation

$$(b_i + q)(b_i - q^{-1}) = 0. \tag{16}$$

$H_N(q)$ is the group algebra of Artin's braid group factored by relation (16). Hecke and Temperley–Lieb algebras are related by the following surjective homomorphism,

$$\varphi : H_N(q) \to TL_N(q): \qquad b_i \mapsto q^{-1} + e_i \qquad \text{and} \qquad b_i^{-1} \mapsto q + e_i. \tag{17}$$

Using this homomorphism, we extend the representation of the Temperley–Lieb algebra (11) to the Hecke algebra

$$\pi_H : H_N(q) \to \operatorname{End} V^{\otimes N}, \qquad b_i \mapsto \pi_H(b_i) := (\pi_{TL} \circ \varphi)(b_i) \tag{18}$$

and obtain

$$b_i \mapsto \pi_H(b_i) := B_i = \begin{pmatrix} q^{-1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & q^{-1} - q & 0 \\ 0 & 0 & 0 & q^{-1} \end{pmatrix}_{i,i+1}. \tag{19}$$

Our motivation to introduce the Hecke algebra will become clear when constructing the new Hilbert space structure with respect to which the Hamiltonian (7) becomes Hermitian. In a purely algebraic context, the Hecke algebra is closely connected to the intertwiners of the quantum group $U_q(sl_2)$ which describes the degenerate eigenspaces of the Hamiltonian (7).

2.2. Quantum group invariance

The spin-chain Hamiltonian (7) possesses several symmetries. In the present context, the most distinguished is its quantum group invariance, which we shall employ in order to define a new Hilbert space structure in which H becomes Hermitian.

Definition 2.3 (quantum group)**.** *The quantum group $U_q(sl_2)$ is a quasi-triangular Hopf algebra generated by the Chevalley–Serre generators $\{s^\pm, q^{\pm s^z}\}$. The latter are subject to the commutation relations*

$$q^{s^z} q^{-s^z} = q^{-s^z} q^{s^z} = 1, \qquad q^{s^z} s^\pm q^{-s^z} = q^{\pm 1} s^\pm, \qquad [s^+, s^-] = [2s^z]_q := \frac{q^{2s^z} - q^{-2s^z}}{q - q^{-1}}. \tag{20}$$

The Hopf algebra structure includes the notions of coproduct $\Delta : U_q(sl_2) \to U_q(sl_2) \otimes U_q(sl_2)$,

$$\Delta(s^\pm) = q^{s^z} \otimes s^\pm + s^\pm \otimes q^{-s^z}, \qquad \Delta\big(q^{\pm s^z}\big) = q^{\pm s^z} \otimes q^{\pm s^z}, \tag{21}$$

antipode $\gamma : U_q(sl_2) \to U_q(sl_2)$

$$\gamma\big(q^{\pm s^z}\big) = q^{\mp s^z}, \qquad \gamma(s^\pm) = -q^{\pm 1} s^\pm, \tag{22}$$

and co-unit $\varepsilon : U_q(sl_2) \to \mathbb{C}$,

$$\varepsilon\left(q^{\pm s^z}\right) = 1, \qquad \varepsilon(s^\pm) = 0. \tag{23}$$

In the following, we will work with the familiar two-dimensional spin-1/2 representation $\pi : U_q(sl_2) \to \text{End } V$, $V = \mathbb{C}^2$, in terms of Pauli matrices, i.e.

$$\pi : \quad s^\pm \mapsto \sigma^\pm \qquad \text{and} \qquad q^{\pm s^z} \mapsto q^{\pm \sigma^z}. \tag{24}$$

The action of the quantum group generators on the spin chain $V^{\otimes N}$ is then obtained via successive application of the coproduct by defining $\Delta_n = (\Delta \otimes 1)\Delta_{n-1}$ starting with $\Delta_2 \equiv \Delta$,

$$\pi_U : U_q(sl_2) \to \text{End } V^{\otimes N}, \qquad x \mapsto \pi^{\otimes N}(\Delta_N(x)), \quad N > 1. \tag{25}$$

We shall denote the images of the Chevalley–Serre generators $\{s^\pm, q^{\pm s^z}\}$ under π_U by capital letters. They read explicitly

$$q^{\pm s^z} \mapsto \pi_U\left(q^{\pm s^z}\right) \equiv q^{\pm S^z}, \qquad S^z = \frac{1}{2}\sum_{i=1}^{N} \sigma_i^z \tag{26}$$

and

$$s^\pm \mapsto \pi_U(s^\pm) \equiv S^\pm = \sum_{i=1}^{N} q^{\frac{\sigma^z}{2}} \otimes \cdots \otimes \underset{i^{\text{th}}}{\sigma^\pm} \otimes q^{-\frac{\sigma^z}{2}} \cdots \otimes q^{-\frac{\sigma^z}{2}}. \tag{27}$$

For q on the unit circle, these generators are non-Hermitian. In fact, one has the relation

$$(S^\pm)^* = S_{\text{op}}^\mp \equiv \pi^{\otimes N}\left(\Delta_N^{\text{op}}(s^\mp)\right) \tag{28}$$

where $S_{\text{op}}^\mp$ are the quantum group generators associated with the opposite coproduct,

$$\Delta^{\text{op}}(s^\pm) = q^{-s^z} \otimes s^\pm + s^\pm \otimes q^{s^z}. \tag{29}$$

We shall refer to the associated Hopf algebra as $U_q^{\text{op}}(sl_2)$. The permuted Hecke algebra generators $r_i = \tau_i b_i$, with τ_i the permutation operator in the ith and $(i+1)$th factors, relate the two coproduct structures (21) and (29),

$$r_i\left(\sigma_i^\pm \otimes q^{-\sigma_{i+1}^z} + q^{\sigma_i^z} \otimes \sigma_{i+1}^\pm\right) = \left(\sigma_i^\pm \otimes q^{\sigma_{i+1}^z} + q^{-\sigma_i^z} \otimes \sigma_{i+1}^\pm\right)r_i. \tag{30}$$

The matrix r_i is referred to as a quantum group intertwiner due to the above relation; it is also commonly called the 'R-matrix'. Both versions of the quantum group appear in the present context: $U_q(sl_2)$ is the symmetry algebra of the Hamiltonian (7), and $U_q^{\text{op}}(sl_2)$ is the symmetry algebra of its Hermitian adjoint H^*,

$$[H, \pi_U(U_q(sl_2))] = \left[H^*, \pi_U\left(U_q^{\text{op}}(sl_2)\right)\right] = 0. \tag{31}$$

These commutation relations are a direct consequence of the following relation which is a quantum analogue of the Schur–Weyl duality.

Theorem 2.1 (Jimbo [21]). *Let* $\pi_U : U_q(sl_2) \to \text{End } V^{\otimes N}$ *and* $\pi_H : H_N(q) \to \text{End } V^{\otimes N}$ *be the representations defined in* (25) *and* (12). *Denote by* $\mathcal{U}'$ *and* $\mathcal{H}'$ *the commutants of the operator algebras* $\mathcal{U} = \pi_U(U_q(sl_2))$ *and* $\mathcal{H} = \pi_H(H_N(q))$ *in* $\text{End } V^{\otimes N}$, *respectively. Then we can identify*

$$\mathcal{U}' = \mathcal{H} \qquad \text{and} \qquad \mathcal{H}' = \mathcal{U}. \tag{32}$$

In the limit $q \to 1$ this gives the familiar Schur–Weyl duality with respect to the symmetric group. Note that in the simple case of sl_2 and $V = \mathbb{C}^2$ considered here, we can specialize in (32) to the Temperley–Lieb algebra. This is due to the fact that for the local spin-1/2

representation (19), and only for this representation, the homomorphism (17) in theorem 2.1 can be 'inverted', i.e. the relation $E_i = q^{-1} - B_i$ yields a representation of the Temperley–Lieb algebra.

The first relation in (31) now follows immediately from theorem 2.1, and the second is obtained when taking the Hermitian adjoint and employing $H(q)^* = H(q^{-1})$ together with (28). Below we will make further use of the duality (32) when discussing the quasi-Hermiticity properties of the Hamiltonian (7) and when introducing a new Hilbert space structure with respect to which H is Hermitian. This concludes our brief review of the algebraic structures relevant for our discussion.

3. PT symmetry on the lattice

We now discuss PT-invariance for the spin chain by introducing parity and time reversal operators on the lattice. Their action is then related to the quantum group invariance of the Hamiltonian and to the transformation properties of a discrete wavefunction ψ.

3.1. Definitions

The Hamiltonian (7) acts on the N-fold tensor product of a two-dimensional space $V = \mathbb{C}^2$ with the orthonormal basis vectors $v_{\frac{1}{2}} = \binom{1}{0}$ and $v_{-\frac{1}{2}} = \binom{0}{1}$. We then have the following orthonormal basis in the Hilbert space $\mathfrak{H} = V^{\otimes N}$,

$$\{|\alpha_1, \ldots, \alpha_N\rangle \equiv v_{\alpha_1} \otimes \cdots \otimes v_{\alpha_N}, \alpha_i = \pm 1/2\}. \tag{33}$$

Definition 3.1 (parity and time-reversal operator). *On the above set of basis vectors we define the linear operator P by setting*

$$P|\alpha_1, \ldots, \alpha_N\rangle = |\alpha_N, \alpha_{N-1}, \ldots, \alpha_1\rangle. \tag{34}$$

In contrast, the operator T acts on the basis vectors as the identity,

$$T|\alpha_1, \ldots, \alpha_N\rangle = |\alpha_1, \ldots, \alpha_N\rangle, \tag{35}$$

but is defined to be antilinear, such that

$$T\lambda|\alpha_1, \ldots, \alpha_N\rangle = \bar{\lambda}|\alpha_1, \ldots, \alpha_N\rangle, \qquad \lambda \in \mathbb{C}. \tag{36}$$

Thus, any matrix A (such as the Hamiltonian A = H) is transformed into its complex conjugate under the adjoint action of T,

$$TAT = \bar{A}. \tag{37}$$

Note that in the particular case considered here the Hamiltonian is symmetric, $H^t = H$, and we therefore have the identity $\bar{H} = H^*$. Together with the crucial relation

$$PHP = H^*, \tag{38}$$

which follows simply from definitions (7) and (34), we obtain as a consequence

$$[PT, H] = 0. \tag{39}$$

Thus, the quantum group invariant *XXZ* Hamiltonian (7) is PT-invariant. However, only if all the eigenfunctions can be chosen to be simultaneous eigenfunctions of the PT-operator can one conclude that the spectrum of H must be real.

Table 1. Commutation relations.

Operator	Temperley–Lieb	Quantum group
Parity reversal	$PE_kP = E_{N-k}^*$	$PS^\pm P = S_{op}^\pm$
Time reversal	$TE_kT = E_k^*$	$TS^\pm T = S_{op}^\pm$
Spin reversal	$RE_kR = E_k^*$	$RS^\pm R = S_{op}^\mp$

3.2. The adjoint PT action on the quantum group and Temperley–Lieb algebra

The Chevalley–Serre generators have the following behaviour under the adjoint action of P and T:

$$PS^\pm P = TS^\pm T = \sum_{i=1}^{N} q^{-\frac{\sigma^z}{2}} \otimes \cdots q^{-\frac{\sigma^z}{2}} \otimes \underset{i^{th}}{\sigma^\pm} \otimes q^{\frac{\sigma^z}{2}} \otimes \cdots q^{\frac{\sigma^z}{2}} = S_{op}^\pm. \quad (40)$$

Thus, the action of PT commutes with that of the quantum group, and as such PT is distinguished from other symmetries of the Hamiltonian. For example, we could have employed the spin-reversal operator

$$R = \prod_{n=1}^{N} \sigma_n^x \quad (41)$$

which leads to additional PR and TR-symmetries,

$$RHR = H^* \qquad \text{and} \qquad [PR, H] = [TR, H] = 0. \quad (42)$$

Notice, however, that the latter do not commute with the quantum group generators,

$$RS^\pm R = S_{op}^\mp, \qquad PRS^\pm PR = RTS^\pm RT = S^\mp. \quad (43)$$

The Temperley–Lieb algebra generators, on the other hand, are not PT-invariant. In the representation (11) they transform according to

$$PE_kP = E_{N-k}^* = TE_{N-k}T \qquad \text{and so} \qquad PTE_k = E_{N-k}PT. \quad (44)$$

For the spin-reversal operator we obtain the identities

$$RE_kR = E_k^*, \qquad PRE_kPR = E_{N-k}, \qquad RTE_kRT = E_k. \quad (45)$$

Note that the PR symmetry is insufficient to introduce a new Hilbert space structure: PR is not a positive operator, whence we cannot use it to define an alternative inner product. In order to arrive at the latter we need the η-operator which we discuss below. Let us summarize the various transformation properties of the respective algebra generators in table 1. In our subsequent discussion we will make frequent use of these commutation relations.

3.3. PT symmetry and Bethe's wavefunction

The term PT symmetry is used in two senses in the quantum mechanics literature: in the weak sense it means simply that $[PT, H] = 0$; in the strong sense the term means that in addition $PT|\psi\rangle \propto |\psi\rangle$ for all eigenvectors $|\psi\rangle$ of H. Clearly, this latter property does not follow from $[PT, H] = 0$. In particular, if the energy eigenvalue of $|\psi\rangle$ is complex, then the antilinearity of T means that the eigenvalue of $PT|\psi\rangle$ is its complex conjugate. If a system displays PT symmetry in the weak but not the strong sense, then it is said to display spontaneous breaking of PT symmetry [10].

In this subsection, we discuss the transformation properties of the eigenvectors of the Hamiltonian H under PT-symmetry. To this end, the formalism of the coordinate Bethe ansatz turns out to be most convenient. This will allow us to determine whether there is a spontaneous breakdown of PT-symmetry and further motivate our existing definition of the parity and time reversal operators by relating them to the transformation behaviour of a 'discrete wavefunction' describing the Bethe vectors.

The coordinate Bethe ansatz for the Hamiltonian (7) has been previously discussed in the literature [14, 17] and we refer the reader to these works for the details of the derivation of the Bethe ansatz equations. We emphasize, however, that PT-symmetry has not been discussed in these works and this is the novel aspect which we want to highlight here.

Before we review the coordinate Bethe ansatz in the context of PT-symmetry, we first introduce the PT-action on discrete wavefunctions. Quite generally, any vector $|\psi\rangle$ in the Hilbert space $\mathfrak{H} = V^{\otimes N}$ with n down-spins is in one-to-one correspondence with a discrete wavefunction $\psi(x_1, \ldots, x_n)$ according to the relation

$$|\psi\rangle = \sum_{1 \leqslant x_1 < \ldots < x_n \leqslant N} \psi(x_1, \ldots, x_n)\sigma_{x_1}^- \cdots \sigma_{x_n}^- |\tfrac{1}{2}, \ldots, \tfrac{1}{2}\rangle, \tag{46}$$

where $|\psi(x_1, \ldots, x_n)|^2$ can be interpreted as the probability to find the n down-spins located at the lattice sites $x_1, \ldots, x_n$. According to our previous definitions (34), (35) the transformation behaviour of the wavefunction under parity reversal is

$$\psi(x_1, \ldots, x_n) \xrightarrow{P} \psi(N+1-x_n, \ldots, N+1-x_1). \tag{47}$$

Time reversal simply amounts to complex conjugation,

$$\psi(x_1, \ldots, x_n) \xrightarrow{T} \bar{\psi}(x_1, \ldots, x_n). \tag{48}$$

These two transformation properties are clearly analogues of the transformation properties of a standard *continuous* wavefunction describing a many-particle system confined to a finite interval on the real line.

The eigenvectors of the Hamiltonian (7) corresponding to highest weight vectors with respect to the quantum group symmetry (31) can be described in terms of Bethe's wavefunction, $\psi = \psi_k$, which can be interpreted as a superposition of reflected plane waves with quasi-momenta $k = (k_1, \ldots, k_n)$, and is defined by

$$\psi_k(x_1, \ldots, x_n) = \sum_{p,\varepsilon}(-1)^{|p|}A\big(\varepsilon_1 k_{p_1}, \ldots, \varepsilon_n k_{p_n}\big)\, \mathrm{e}^{\mathrm{i}(\varepsilon_1 k_{p_1} x_1 + \cdots + \varepsilon_n k_{p_n} x_n)}. \tag{49}$$

The sum runs over all permutations $p = (p_1, \ldots, p_n) \in S_n$ of the index set $(1, \ldots, n)$ as well as all possible sign changes $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)$, $\varepsilon_i = \pm 1$ (due to the reflection at the boundaries of the finite spin chain). The symbol $|p|$ indicates the sign ± 1 of the permutation, with the choice $|(1, 2, \ldots, n)| = +1$. It is shown in [14] that the coefficients $A(k_1, \ldots, k_n)$ have the form

$$A(k_1, \ldots, k_n) = \prod_j \beta(-k_j) \prod_{j<l} B(-k_j, k_l)\, \mathrm{e}^{-\mathrm{i}k_l}, \tag{50}$$

where we have introduced the functions

$$\beta(k) = (1 - q\, \mathrm{e}^{-\mathrm{i}k})\, \mathrm{e}^{\mathrm{i}(N+1)k} \tag{51}$$

and

$$B(k_1, k_2) = s(-k_1, k_2)s(k_2, k_1), \qquad s(k_1, k_2) := (1 - (q + q^{-1})\, \mathrm{e}^{\mathrm{i}k_1} + \mathrm{e}^{\mathrm{i}(k_1+k_2)}). \tag{52}$$

For later use we note the simple identities (note that we have $\bar{q} = q^{-1}$)

$$\overline{\beta(-\bar{k})} = -q^{-1} \, \mathrm{e}^{\mathrm{i}(2N+1)k} \beta(-k), \qquad \overline{B(-\bar{k}_1, \bar{k}_2)} = B(-k_2, k_1) \, \mathrm{e}^{-\mathrm{i}(k_1+k_2)} \frac{s(-k_2, k_1)}{s(k_1, -k_2)}. \qquad (53)$$

In order that $|\psi_{\boldsymbol{k}}\rangle$ be an eigenvector, it is necessary that the quasi-momenta $k_1, \ldots, k_n$ satisfy the Bethe ansatz equations

$$\mathrm{e}^{2\mathrm{i}Nk_j} = \prod_{l \neq j} \frac{B(-k_j, k_l)}{B(k_j, k_l)}. \qquad (54)$$

The corresponding eigenvalue of the Hamiltonian is

$$\lambda = (N-1)\Delta_+ + 4 \sum_{j=1}^{n} (\cos k_j - \Delta_+). \qquad (55)$$

The analytic solutions to the Bethe ansatz equations are not known. However, we can discuss in abstract terms the action of parity and time reversal on the Bethe wavefunction. We have

$$PT\psi_{\boldsymbol{k}}(x_1, \ldots, x_n) = \sum_{p, \varepsilon} (-1)^{|p|} \overline{A\big(\varepsilon_1 k_{p_1}, \ldots, \varepsilon_n k_{p_n}\big)} \, \mathrm{e}^{-\mathrm{i}(\varepsilon_1 \bar{k}_{p_1}(N+1-x_n) + \cdots + \varepsilon_n \bar{k}_{p_n}(N+1-x_1))}$$

$$= -\sum_{p, \varepsilon} (-1)^{|p|} \overline{A\big(\varepsilon_n k_{p_n}, \ldots, \varepsilon_1 k_{p_1}\big)} \, \mathrm{e}^{-\mathrm{i}(N+1)(\varepsilon_1 \bar{k}_{p_1} + \cdots + \varepsilon_n \bar{k}_{p_n})} \, \mathrm{e}^{\mathrm{i}(\varepsilon_1 \bar{k}_{p_1} x_1 + \cdots + \varepsilon_n \bar{k}_{p_n} x_n)}.$$

The minus sign comes from the sign difference of the two permutations $(p_1, \ldots, p_n)$ and $(p_n, \ldots, p_1)$. Now let us assume that the Bethe roots k_i consist of m complex pairs $(k_i, k_{i'})$ of the form $\bar{k}_i = \pm k_{i'}$, and $n - 2m$ real roots. This assumption is certainly consistent with the reality of the spectrum due to (55). Under this assumption, we can write

$$PT\psi_{\boldsymbol{k}}(x_1, \ldots, x_n)$$
$$= (-)^{1+m} \sum_{p, \varepsilon} (-1)^{|p|} \overline{A\big(\varepsilon_n \bar{k}_{p_n}, \ldots, \varepsilon_1 \bar{k}_{p_1}\big)} \, \mathrm{e}^{-\mathrm{i}(N+1)(\varepsilon_1 k_{p_1} + \cdots + \varepsilon_n k_{p_n})} \, \mathrm{e}^{\mathrm{i}(\varepsilon_1 k_{p_1} x_1 + \cdots + \varepsilon_n k_{p_n} x_n)}.$$

$$(56)$$

It follows that we have $PT\psi_{\boldsymbol{k}}(x_1, \ldots, x_n) \propto \psi_{\boldsymbol{k}}(x_1, \ldots, x_n)$ if

$$A(k_1, \ldots, k_n) \propto \overline{A(\bar{k}_n, \ldots, \bar{k}_1)} \, \mathrm{e}^{-\mathrm{i}(N+1)(k_1 + \cdots k_n)} \qquad (57)$$

for any set of $\boldsymbol{k} = (k_1, \ldots, k_n)$ satisfying the Bethe ansatz equations (54). This is a consequence of the following proposition.

Proposition 3.1. *If $k_1, \ldots, k_n$ satisfy the Bethe equations (54), we have*

$$\overline{A(\bar{k}_1, \ldots, \bar{k}_n)} = (-q)^{-n} \, \mathrm{e}^{\mathrm{i}(N+1)(k_1 + \cdots + k_n)} A(k_n, \ldots, k_1). \qquad (58)$$

Proof. Using the above identities (53) for $\bar{\beta}$ and $\bar{B}$, we have

$$\overline{A(\bar{k}_1, \ldots, \bar{k}_n)} = (-q)^{-n} \, \mathrm{e}^{\mathrm{i}(2N+1)(k_1 + \cdots + k_n)} \prod_j \beta(-k_j) \prod_{j<l} B(-k_l, k_j) \, \mathrm{e}^{-\mathrm{i}k_j} \frac{s(-k_l, k_j)}{s(k_j, -k_l)}. \qquad (59)$$

The next step is to take the product of the Bethe equations over all $j = 1, \ldots, n$. This gives

$$\mathrm{e}^{2\mathrm{i}N(k_1 + \cdots + k_n)} = \prod_j \prod_{l \neq j} \frac{s(k_j, k_l)s(k_l, -k_j)}{s(-k_j, k_l)s(k_l, k_j)} = \prod_j \prod_{l \neq j} \frac{s(k_l, -k_j)}{s(-k_j, k_l)},$$

$$= \prod_{j<l} \frac{s(k_l, -k_j)}{s(-k_j, k_l)} \prod_{j<l} \frac{s(k_j, -k_l)}{s(-k_l, k_j)} = \prod_{j<l} \frac{s^2(k_j, -k_l)}{s^2(-k_l, k_j)}, \qquad (60)$$

where we have used the identity $s(k_1, k_2) = e^{i(k_1+k_2)} s(-k_2, -k_1)$ in the last step. Then we have

$$\prod_{j<l} \frac{s(-k_l, k_j)}{s(k_j, -k_l)} = e^{-iN(k_1+\cdots+k_n)}. \tag{61}$$

The left-hand side of this expression appears in equation (59), and after substituting we arrive at

$$\overline{A(\bar{k}_1, \ldots, \bar{k}_n)} = (-q)^{-n} e^{i(N+1)(k_1+\cdots+k_n)} \prod_j \beta(-k_j) \prod_{j<l} B(-k_l, k_j) e^{-ik_j}$$

$$= (-q)^{-n} e^{i(N+1)(k_1+\cdots+k_n)} A(k_n, \ldots, k_1) \tag{62}$$

$$\square$$

If follows that for each Bethe vector with n down spins (i.e. S_z eigenvalue $N/2 - n$), m complex pairs $(k_i, k_{i'})$ of the form $\bar{k}_i = \pm k_{i'}$ and $n - 2m$ real roots, we have

$$PT\psi_{\boldsymbol{k}}(x_1, \ldots, x_n) = (-1)^{1+m}(-q)^{-n}\psi_{\boldsymbol{k}}(x_1, \ldots, x_n) \tag{63}$$

and hence

$$PT|\psi_{\boldsymbol{k}}\rangle = (-1)^{1+m}(-q)^{-n}|\psi_{\boldsymbol{k}}\rangle. \tag{64}$$

Thus, for this particular set of eigenvectors at least, and—because of (40)—for their associated degenerate eigenspaces, we can conclude that PT-symmetry is not spontaneously broken. However, since it is generally difficult to verify the precise nature of the Bethe roots (i.e. whether only real or complex pairs of them occur) as well as to rigorously prove that the Bethe ansatz yields the complete set of eigenvectors, alternative arguments have to be employed to prove the reality of the spectrum of (7).

4. Exact construction of the quasi-Hermiticity operator η

As outlined in the introduction, we need to find a positive definite, Hermitian and invertible operator η satisfying (2) in order to define a new Hilbert space structure (3) with respect to which the Hamiltonian (7) becomes Hermitian. For many non-Hermitian systems in the literature, this has been achieved by using bi-orthonormal systems of Hamiltonian eigenvectors. While we will not follow this approach in our construction of η, because the solutions of the Bethe ansatz equations (54) are in general unknown, let us briefly make contact with this method as we will repeatedly refer to it in our subsequent discussion.

To start with, we note that the existence of a map η with the aforementioned properties implies that H and H^* have real spectrum. However, the converse of this statement is in general *not* true. Suppose we are given a finite-dimensional non-Hermitian Hamiltonian H, such that H and H^* have purely real spectra, $\text{Spec } H = \text{Spec } H^* \subset \mathbb{R}$. Then there exist two corresponding sets of eigenvectors $\{\phi_\lambda\}_{\lambda \in \text{Spec } H}$ of H and $\{\psi_\lambda\}_{\lambda \in \text{Spec } H}$ of H^* such that

$$H\phi_\lambda = \lambda\phi_\lambda \qquad \text{and} \qquad H^*\psi_\lambda = \lambda\psi_\lambda. \tag{65}$$

Making the *additional* assumption that the eigenvectors can be normalized such that the relations

$$\langle\phi_\lambda, \psi_{\lambda'}\rangle = \delta_{\lambda,\lambda'} \qquad \text{and} \qquad \sum_{\lambda \in \text{Spec } H} |\phi_\lambda\rangle\langle\psi_\lambda| = \mathbf{1} \tag{66}$$

both hold, one can then define η to be the following sum over projectors

$$\eta = \sum_{\lambda \in \text{Spec } H} |\psi_\lambda\rangle\langle\psi_\lambda| = \left(\sum_{\lambda \in \text{Spec } H} |\phi_\lambda\rangle\langle\phi_\lambda|\right)^{-1}. \tag{67}$$

The above map η satisfies all necessary requirements by construction. We stress, however, that the crucial assumption concerning the existence of a bi-orthonormal system of eigenvectors satisfying (66) is not always satisfied.

In particular, the spin-chain Hamiltonian (7) provides a counterexample. Namely, if we choose q to be a primitive root of unity, then one can verify that the Hamiltonian possesses non-trivial Jordan blocks. As a result there always exist eigenvalues $\lambda \in \operatorname{Spec} H$ for which the associated eigenvectors ϕ_λ, ψ_λ are orthogonal,

$$\langle \phi_\lambda, \psi_\lambda \rangle = 0. \tag{68}$$

The connection between such states and non-trivial Jordan blocks has been discussed, for example, in [15, 16]. The occurrence of such states in the present context can be understood in terms of representation theory [17]. Due to (68), the assumption (66) is violated and one only finds a positive semi-definite matrix η, $\eta \geqslant 0$, when q is a root of unity. The solution to this problem of defining a Hermitian version of the quantum group invariant *XXZ* Hamiltonian at roots of unity is to remove the aforementioned subset of states from the Hilbert space, making η positive definite, $\eta > 0$, and, consequently, the Hamiltonian diagonalizable. This procedure is known as 'quantum group reduction at roots of unity'. This reduction procedure has been developed previously in the literature on integrable systems [19]. The new aspect of our discussion here is its relation to the ideas of quasi-Hermiticity. Developing this connection will put us into the position to present in the last part of this paper a novel algebraic formulation of the Hilbert space structure which makes (7) Hermitian.

4.1. The path basis

In order to reduce the state space we first introduce a different set of basis vectors. The new set of basis vectors which we are going to construct is dictated by the quantum group invariance of the Hamiltonian and has the advantage that the set of 'problematic' states (68) can be easily identified. For the moment, we keep $q = \exp(i\pi/r)$ generic, but shall specialize below to integer values $r \geqslant 3$.

The new basis states will be obtained by successively decomposing tensor products of $U_q(sl_2)$ representations into the finite-dimensional irreducible representations $\pi_j : U_q(sl_2) \to \operatorname{End} \mathbb{C}^{2j+1}$ with $j \in \frac{1}{2}\mathbb{N}$. Up to isomorphism the latter are given by

$$\pi_j(s^\pm)|j, m\rangle = \sqrt{[j \mp m]_q [j \pm m + 1]_q}\, |j, m \pm 1\rangle,$$
$$\pi_j(q^{s^z})|j, m\rangle = q^m |j, m\rangle, \qquad m = -j, -j+1, \ldots, j-1, j. \tag{69}$$

In analogy with the terminology used for sl_2, the half-integer j labelling the representation is referred to as 'spin'. Following [19, 18], we now introduce a 'path basis' using the q-deformed Clebsch–Gordan (CG) coefficients defined implicitly via the embedding

$$\iota_{12} : \pi_J \hookrightarrow \pi_{j_1} \otimes \pi_{j_2}, \qquad |J, M\rangle \hookrightarrow \sum_{m_1+m_2=M} \begin{vmatrix} j_1 & j_2 & J \\ m_1 & m_2 & M \end{vmatrix}_q |j_1, m_1\rangle \otimes |j_2, m_2\rangle. \tag{70}$$

The relevant CG coefficients for the spin-1/2 chain are computed via the action of the coproduct (see appendix C),

$$\begin{vmatrix} j & \frac{1}{2} & j + \frac{1}{2} \\ m & \alpha & m + \alpha \end{vmatrix}_q = q^{-\alpha j + \frac{m}{2}} \left(\frac{[j + 2\alpha m + 1]}{[2j + 1]} \right)^{\frac{1}{2}} \tag{71}$$

and

$$\begin{vmatrix} j & \frac{1}{2} & j - \frac{1}{2} \\ m & \alpha & m + \alpha \end{vmatrix}_q = 2\alpha q^{\alpha(j+1) + \frac{m}{2}} \left(\frac{[j - 2\alpha m]}{[2j + 1]} \right)^{\frac{1}{2}}. \tag{72}$$

Now let $\boldsymbol{j} = (j_0, j_1, j_2, \ldots, j_N)$ be a path on the sl_2-Bratelli diagram, i.e. the set of sequences specified as follows:

$$\Gamma = \{\boldsymbol{j} = (j_0, j_1, j_2 \ldots, j_N) | j_0 = 0, \ j_k \geqslant 0, \ j_{k+1} = j_k \pm 1/2\}. \tag{73}$$

Here we have followed the common convention to root the paths at $j_0 = 0$ which forces $j_1 = 1/2$. Next, we define the vectors

$$|\boldsymbol{j}, m\rangle = \sum_{|\boldsymbol{\alpha}|=m} |\boldsymbol{\alpha}\rangle \langle \boldsymbol{\alpha} | \boldsymbol{j}, m\rangle, \qquad m = -j_N, -j_N + 1, \ldots, 0, \ldots, j_N \tag{74}$$

with

$$\langle \boldsymbol{\alpha} | \boldsymbol{j}, m\rangle = \prod_{k=1}^{N-1} \left| \begin{matrix} j_k & \frac{1}{2} & j_{k+1} \\ \sum_{i \leqslant k} \alpha_i & \alpha_{k+1} & \sum_{i \leqslant k+1} \alpha_i \end{matrix} \right|_q, \qquad m = |\boldsymbol{\alpha}| := \sum_{k=1}^{N} \alpha_k = S^z. \tag{75}$$

As long as q is not a root of unity the above basis is well defined. If r is an integer $\geqslant 3$, however, one has to constrain the set of allowed paths to the restricted Bratelli diagram

$$\Gamma^{(r)} := \{\boldsymbol{j} \in \Gamma | 2j_k + 1 < r, k = 1, \ldots, N\}. \tag{76}$$

This restriction ensures that no singularities or cancellations occur in the CG coefficients due to the factors $[2j_k + 1]_q = [r]_q = 0$. It is precisely the reduction of the state space by the constraint (76) which removes the states (68) mentioned above in the context of quasi-Hermiticity. As we will see below, we can then explicitly construct a positive map η on the reduced state space.

4.2. Action of the Temperley–Lieb algebra in the path basis

The introduction of the path basis is not only motivated by aspects of quasi-Hermiticity, but is rather natural from an algebraic point of view. It allows us to factor out the quantum group action which commutes with the Hamiltonian and spans its degenerate eigenspaces. In fact, given a fixed path $\boldsymbol{j}$ on the Bratelli diagram the action of the quantum group $U_q(sl_2)$ will not change this path but only modify the corresponding 'magnetic quantum number' m in the associated path state (74), i.e. each path $\boldsymbol{j} = (j_0 = 0, j_1 = 1/2, j_2, \ldots, j_N) \in \Gamma$ corresponds to an irreducible quantum group module of spin j_N given by (69).

The Hamiltonian, on the other hand, can only mix paths with the same end point j_N and leaves m unchanged due to (31). The same holds true for the generators of the Temperley–Lieb algebra. Both assertions follow immediately from the quantum version of Schur–Weyl duality (32). They can be explicitly verified by computing the action of the Temperley–Lieb generators (11) in the path basis from (71), (72) and (74) (see appendix C for the relevant identities). One finds for $k = 2, \ldots, N-1$ the following result,

$$E_k|\boldsymbol{j}, m\rangle = \delta_{j_{k-1}, j_{k+1}} \sum_{j'=j_{k-1}\pm 1/2} \frac{\sqrt{[2j_k + 1]_q [2j' + 1]_q}}{(-)^{j_k - j' + 1} [2j_{k-1} + 1]_q} |j_0, j_1, \ldots j_{k-1}, j', j_{k+1}, \ldots j_N, m\rangle, \tag{77}$$

where $|\boldsymbol{j}, m\rangle = 0$ if $j_i < 0$ for some i. Note that for $k = 1$ the formula (77) therefore simplifies to

$$E_1|\boldsymbol{j}, m\rangle = -\delta_{0, j_2}[2]_q|\boldsymbol{j}, m\rangle, \tag{78}$$

where we have used the expressions

$$\left| \begin{matrix} \frac{1}{2} & \frac{1}{2} & 1 \\ \alpha_1 & \alpha_2 & m \end{matrix} \right|_q = q^{\frac{\alpha_1 - \alpha_2}{2}} \left(\frac{\left[\frac{3}{2} + 2\alpha_1\alpha_2\right]}{[2]} \right)^{\frac{1}{2}}, \qquad \left| \begin{matrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \alpha_1 & \alpha_2 & 0 \end{matrix} \right|_q = -2\alpha_1 q^{-\alpha_1}/[2]^{\frac{1}{2}}. \tag{79}$$

Table 2. Dimensions $\dim \Gamma_j$ and $\dim \Gamma_j^{(5)}$ for different chains of length N.

$N \backslash j$	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$	3	$\frac{7}{2}$	4	$\frac{9}{2}$	5
0	1										
1		1									
2	1		1								
3		2		1							
4	2		3		1						
5		5		4		1					
6	5		9		5		1				
7		14		14		6		1			
8	14		28		20		7		1		
9		42		48		27		8		1	
10	42		90		75		35		9		1

$N \backslash j$	0	$\frac{1}{2}$	1	$\frac{3}{2}$
0	1			
1		1		
2	1		1	
3		2		1
4	2		3	
5		5		3
6	5		8	
7		13		8
8	13		21	
9		34		21
10	34		55	

Thus, E_1 is a diagonal matrix in the path basis. From expression (77), one can now directly read off the previously stated properties of the action of the Temperley–Lieb algebra and the Hamiltonian. As far as the Temperley–Lieb action is concerned, one may disregard the magnetic quantum number m in (74) and concentrate on the subspaces

$$\Gamma_j := \{ \boldsymbol{j} \in \Gamma | \boldsymbol{j} = (0, 1/2, j_2, \ldots, j_{N-1}, j_N = j) \} \tag{80}$$

with the fixed end point j which according to (77) are invariant. In an analogous fashion we define for $q = \exp(i\pi/r)$ with r integer the set

$$\Gamma_j^{(r)} := \Gamma^{(r)} \cap \Gamma_j. \tag{81}$$

The representations Γ_j and $\Gamma_j^{(r)}$ can respectively be shown to be equivalent to the finite-dimensional irreducible representations of the Temperley–Lieb algebra at generic q and at roots of unity $q^r = -1$ given, for example, in [22–25] and references therein. We discuss an alternative, graphical description of the irreducible representations of $TL_N(q)$ in appendix A.

When decomposing the Hilbert space $V^{\otimes N}$ into the irreducible representations π_j of the quantum group for generic q, the following multiplicities μ_j occur which coincide with the dimension of the path space Γ_j,

$$\dim \Gamma_j = \mu_j := \binom{N}{N/2 - j} - \binom{N}{N/2 + j + 1}. \tag{82}$$

For $q = \exp(i\pi/r)$ with r integer $\geqslant 3$, the dimensions of the irreducible representations $\Gamma_j^{(r)}$ are obtained via the formula,

$$\dim \Gamma_j^{(r)} = \sum_{k=-\infty}^{\infty} \mu_{j+rk}, \tag{83}$$

where the sum always turns out to contain only a finite number of non-vanishing terms, since $\binom{m}{n} = 0$ for $n < 0$ or $n > m$. An illustration of the multiplicities is given in table 2.

4.3. Path basis construction of η at roots of unity

We are now in the position to construct the map η described in the introduction which will allow us to establish quasi-Hermiticity for the Hamiltonian (7). As a preparatory step, we first introduce the path basis with respect to the Hermitian adjoint Hamiltonian H^*. Using the time

reversal operator (i.e. complex conjugation with respect to the spin basis (33)) we define the conjugate path basis

$$|\boldsymbol{j}, m\rangle_T := T|\boldsymbol{j}, m\rangle = \sum_{|\alpha|=m} |\alpha\rangle \, \overline{\langle\alpha|\boldsymbol{j}, m\rangle}, \qquad \boldsymbol{j} \in \Gamma, \qquad m = -j_N, -j_N + 1, \ldots, j_N.$$

(84)

Using the unitarity relation

$$\sum_{m,\alpha} \begin{vmatrix} j & \frac{1}{2} & j' \\ m & \alpha & m' \end{vmatrix}_q \begin{vmatrix} j & \frac{1}{2} & j'' \\ m & \alpha & m'' \end{vmatrix}_q = \delta_{j',j''}\delta_{m',m''}$$

(85)

we have the following identities:

$$_T\langle\boldsymbol{j}, m|\boldsymbol{j}', m'\rangle = \delta_{m,m'}\prod_k \delta_{j_k,j'_k} \qquad \text{and} \qquad \mathbf{1} = \sum_{\boldsymbol{j},m} |\boldsymbol{j}, m\rangle_T \langle\boldsymbol{j}, m|. \quad (86)$$

The above relations hold for all values of q on the unit circle. In particular, the completeness relation (the second identity in (86)) continues to be true when q is a root of unity, $q = \exp(\mathrm{i}\pi/r)$ with r integer $\geqslant 3$, and the path space is reduced to (76). For the remainder of this section we shall assume that we are at such a special root of unity value.

Definition 4.1 (η at roots of 1). *Let $q = \mathrm{e}^{\mathrm{i}\pi/r}$ with $r > 2$ and integer. Then we define the quasi-Hermiticity operator η to be*

$$\eta = \sum_{\boldsymbol{j},m} |\boldsymbol{j}, m\rangle_{T\,T}\langle\boldsymbol{j}, m|,$$

(87)

where the sum ranges over all restricted paths $\boldsymbol{j} \in \Gamma^{(r)}$ defined in (76) and m over the values given in (84).

By definition, η is positive definite. Its expression in terms of projectors onto path states is reminiscent of similar expressions in terms of bi-orthonormal systems of eigenvectors as they can be found in the literature on PT-symmetry and quasi-Hermiticity; compare with (65), (66) and (67). We wish to stress, however, that the path states are *not* eigenvectors of the Hamiltonian and that they are explicitly given through the CG coefficients (71), (72) and (84). Thus, we have a *non-perturbative, exact and explicit* expression for the quasi-Hermiticity operator η without having to rely on the construction of the eigenvectors of the Hamiltonian. To emphasize this point even further, we explicitly state the matrix elements of η in the local spin basis,

$$\langle\alpha|\eta|\beta\rangle = \sum_{\boldsymbol{j},m} \overline{\langle\alpha|\boldsymbol{j}, m\rangle} \, \langle\beta|\boldsymbol{j}, m\rangle$$

$$= \sum_{\boldsymbol{j},m} \prod_{k=1}^{M-1} \overline{\begin{vmatrix} j_k & \frac{1}{2} & j_{k+1} \\ m_k & \alpha_{k+1} & m_{k+1} \end{vmatrix}_q} \begin{vmatrix} j_k & \frac{1}{2} & j_{k+1} \\ m'_k & \beta_{k+1} & m'_{k+1} \end{vmatrix}_q.$$

(88)

It remains to show that the map η defined by (87) intertwines the Hamiltonian (7) with its Hermitian adjoint. In fact, we find that it obeys more stringent conditions.

Proposition 4.1. *As before, let $q = \exp(\mathrm{i}\pi/r)$ with r an integer >2. Then the map η defined in (87) satisfies the identity*

$$\eta E_k = E_k^* \eta.$$

(89)

Here $\{E_k\}_{k=1}^{N-1}$ are the Temperley–Lieb generators (13) in the representation (77) and under the restriction (76). In addition, the following equalities hold for the quantum group generators:

$$\eta S^{\pm} = (S^{\mp})^* \eta = S_{op}^{\pm} \eta \qquad and \qquad [\eta, S^z] = 0. \tag{90}$$

Again these identities are valid only after the reduction of the state space according to (76) has been imposed.

Proof. In order to derive the first identity we note that the matrix elements of the Temperley–Lieb generators in (77) are real numbers as long as all q-integers appearing in the above equation (77) are positive. This is guaranteed by the choice of q and the restriction of the paths to the Bratelli diagram $\Gamma^{(r)}$ in (76). This explains the first equality in the sequence

$$\eta E_k |\boldsymbol{j}, m\rangle = T E_k |\boldsymbol{j}, m\rangle = E_k^* T |\boldsymbol{j}, m\rangle = E_k^* \eta |\boldsymbol{j}, m\rangle. \tag{91}$$

The second equality follows from the observation that the Temperley–Lieb generators are represented as symmetric matrices. The final equality arises simply from the definition (87). Together with the fact that the path states form a basis this proves (89). In a similar fashion one proves the second identity for the quantum group generators. □

We then have as a trivial consequence of the above proposition the desired property

$$\eta H = H^* \eta, \qquad H = \sum_{k=1}^{N-1} E_k. \tag{92}$$

Thus, we have also demonstrated that H is indeed quasi-Hermitian and that (87) defines the physically relevant inner product (3) with respect to which H is Hermitian. This is particularly important for the calculation of physically relevant quantities such as correlation functions where one considers matrix elements of local operators [26]. While the expression (88) is especially convenient for numerical computations, an alternative formulation in terms of the relevant algebras would be desirable in order to apply more powerful mathematical techniques. In light of (89) and (90), we can immediately conclude that η cannot be expressed in terms of the quantum group or Temperley–Lieb algebra (see (32)). We therefore turn our attention to the C-operator.

5. The *C*-operator

In the context of PT-symmetry, Bender and collaborators introduced the C-operator in order to construct a well-defined inner product with respect to which the Hamiltonian becomes Hermitian (for references see [6]). It is now understood that this approach is a special case of quasi-Hermiticity.

Definition 5.1 [the C-operator]. *Given a positive, Hermitian and invertible map $\eta : \mathfrak{H} \to \mathfrak{H}$ with $\eta H = H^* \eta$, the C-operator is defined to be the linear map*

$$C = P\eta, \tag{93}$$

where P is the previously defined parity operator which is assumed to obey (38).

An immediate consequence of the above definition is the relation

$$[H, C] = 0. \tag{94}$$

It should be clear that the choice of the parity operator in (93) is only dictated by convenience. For instance, in the present case—due to (42)—we might equally well choose the spin-reversal operator R instead of P which leads to a second, alternative definition.

Definition 5.2 (the C′-operator). *For given η as in the previous definition, we set*

$$C' = R\eta. \tag{95}$$

Again we have that $[H, C'] = 0$. In contrast, the choice of the time reversal operator T for the definition of C would not be on the same footing, because T is antilinear. In the literature on PT-symmetry, one usually finds the additional requirement that C is an involution, i.e.

$$C^2 = 1 \tag{96}$$

or equivalently that

$$P\eta P = \eta^{-1}. \tag{97}$$

In many examples this turns out to be true. In particular, if (38) holds and a bi-orthonormal eigensystem (65), (66) can be chosen such that $P\phi_\lambda = \psi_\lambda$, the properties (96) and (97) immediately follow from (67). Nevertheless, (96) is not a fundamental property necessary to ensure that the inner product (3) is well defined. For this reason we have not included this property in the definition of C. However, we will show below that (96) does indeed hold true in the present construction and that the analogous relation is satisfied by C' as well.

Our motivation to consider the two aforementioned C-operators becomes clear when looking at their commutation relations. As we well discuss below, the operator C commutes with the quantum group action while C' commutes with the Temperley–Lieb action. We will use these commutation relations to describe the properties of C, C' and give algebraic construction for both.

5.1. Properties and identities of the C-operators

We start the discussion with the operator C' as its action in the path basis is considerably simpler than the action of C. In the second step, we shall then use these results to find an elegant algebraic expression for the operator C in terms of the Hecke algebra.

Theorem 5.1. *Let $q = \exp(i\pi/r)$ with r integer $\geqslant 3$ and η be the previously defined sum over projectors in the path basis (87). Set $C' = R\eta$ with R the spin-reversal operator. Then*

$$C'|\boldsymbol{j}, m\rangle = (-)^{\frac{N}{2} - j_N}|\boldsymbol{j}, -m\rangle, \tag{98}$$

where j_N is the endpoint of the path $\boldsymbol{j}$. Thus, we have in particular that $C'^2 = 1$ or equivalently

$$R\eta R = \eta^{-1}. \tag{99}$$

According to (69) and (98) the operator C' can be expressed on $\Gamma_j^{(r)}$ in terms of the quantum group generators as

$$C'|_{\Gamma_j^{(r)}} = (-)^{\frac{N}{2} - j} \sum_{m \in \frac{1}{2}\mathbb{N}} \frac{[j - m]_q!}{[j + m]_q!} \frac{(S^-)^{2m}\delta_{S_z,m} + (S^+)^{2m}\delta_{S_z,-m}}{2^{\delta_{0,m}}}. \tag{100}$$

This gives an expression for C' which is independent of the path basis.

Proof. First we note from (89) and (45) that $C' = R\eta$ commutes with the Temperley–Lieb algebra and hence we can conclude from (32) that $C' \in \mathcal{U}$. Since each subspace $\Gamma_j^{(r)}$ of restricted paths with the same endpoint $j_N = j$ forms an irreducible, faithful representation of the Temperley–Lieb algebra, it suffices to compute the action of C' on $|\boldsymbol{j}', m\rangle$ for some special path $\boldsymbol{j}' \in \Gamma_j^{(r)}$ in order to infer its action on any path state $|\boldsymbol{j}, m\rangle, \boldsymbol{j} \in \Gamma_j^{(r)}$. In other words, C' can at most change the magnetic quantum number m but not the actual path $\boldsymbol{j}$ in a path state $|\boldsymbol{j}, m\rangle$.

For given j_N let us pick the path $\boldsymbol{j}'$ on the Bratelli diagram which alternates a maximal number of times between $j = 0$ and $j = 1/2$ before increasing monotonically to $j = j_N$ (for example, if $N = 6$ and $j_6 = 2$, we would choose $\boldsymbol{j}' = (0, 1/2, 0, 1/2, 1, 3/2, 2)$). Then the path states $|\boldsymbol{j}', \pm j_N\rangle$ consist of the following linear combination of vectors in the spin basis,

$$|\boldsymbol{j}', \pm j_N\rangle = \sum_{\alpha_k} \Big|\alpha_1, -\alpha_1, \ldots, \alpha_{N-2j_N}, -\alpha_{N-2j_N}, \underbrace{\pm\tfrac{1}{2}, \ldots, \pm\tfrac{1}{2}}_{2j_N}\Big\rangle \prod_{k=1}^{\frac{N}{2}-j_N} \left(-\frac{2\alpha_k q^{-\alpha_k}}{[2]_q^{1/2}}\right). \quad (101)$$

Here we have used the following identities for the Clebsch–Gordan coefficients in the path basis expansion (74),

$$\prod_{k=1}^{\frac{N}{2}-j_N} \begin{vmatrix} \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ \alpha_k & -\alpha_k & 0 \end{vmatrix}_q \begin{vmatrix} 0 & \tfrac{1}{2} & \tfrac{1}{2} \\ 0 & \alpha_{k+1} & \alpha_{k+1} \end{vmatrix}_q = \prod_{k=1}^{\frac{N}{2}-j_N} \left(-\frac{2\alpha_k q^{-\alpha_k}}{[2]_q^{1/2}}\right) \quad (102)$$

and

$$\prod_{k=0}^{2j_N-1} \begin{vmatrix} \tfrac{k}{2} & \tfrac{1}{2} & \tfrac{k+1}{2} \\ \pm\tfrac{k}{2} & \pm\tfrac{1}{2} & \pm\tfrac{k+1}{2} \end{vmatrix}_q = 1. \quad (103)$$

From the above expressions one now easily verifies that

$$C'|\boldsymbol{j}', j_N\rangle = R|\boldsymbol{j}', j_N\rangle_T = (-)^{\frac{N}{2}-j_N}|\boldsymbol{j}', -j_N\rangle. \quad (104)$$

But (90) and (43) now imply

$$\begin{aligned} C'|\boldsymbol{j}', m\rangle &= \mathcal{N}_m C'(S^-)^{j_N-m}|\boldsymbol{j}', j_N\rangle = \mathcal{N}_m(S^+)^{j_N-m}C'|\boldsymbol{j}', j_N\rangle \\ &= (-)^{\frac{N}{2}-j_N}\mathcal{N}_m(S^+)^{j_N-m}|\boldsymbol{j}', -j_N\rangle = (-)^{\frac{N}{2}-j_N}|\boldsymbol{j}', -m\rangle. \end{aligned} \quad (105)$$

Here $\mathcal{N}_m = \sqrt{[j_N+m]_q!/[2j_N]_q![j_N-m]_q!}$ is some unimportant normalization constant (see (69)). Expression (100) now also follows from this result. Note that (100) is consistent with the quantum Schur–Weyl duality (32), $C' \in \mathcal{U}$, since the Kronecker δ-functions can be rewritten in terms of the quantum group generators $q^{\pm S^z}$,

$$\delta_{S_z, \pm m} = r^{-1} \sum_{k=1}^{r} q^{4(m \mp S^z)k}. \quad (106)$$

$\square$

From the above theorem we infer that the action of C' is surprisingly simple; a result which is not obvious given the expression (87) involving a sum of projectors. However, we stress that the simple action (98) is special to the path basis construction.

We now state the analogous result for the C-operator and give its explicit algebraic form.

Theorem 5.2. *Let η be defined as before and set $C = P\eta$. Then we have that*

$$[C, C'] = 0 \qquad and \qquad C^2 = 1. \quad (107)$$

Furthermore, upon restriction to the invariant subspaces $\Gamma_j^{(r)}$ the following operator identity holds:

$$C|_{\Gamma_j^{(r)}} = \chi_j \mathcal{B}, \qquad \chi_j \in \mathbb{C}. \quad (108)$$

Here $\mathcal{B}$ denotes the image of the following special braid β under the representation (19) respectively (77) induced via (17),

$$\beta = \beta_1 \beta_2 \cdots \beta_{N-1}, \qquad \beta_n = b_n b_{n-1} \cdots b_1. \quad (109)$$

Proof. From the transformations (90) and (40) we infer that the C-operator is quantum group invariant, $[C, \mathcal{U}] = 0$. That is, according to the quantum analogue of Schur–Weyl duality (32) we must have $C \in \mathcal{H}$. We already saw in the proof of the previous theorem that $[C', \mathcal{H}] = 0$, whence $C' \in \mathcal{U}$. Hence, the first assertion, $[C, C'] = 0$, trivially follows from (32). But due to the fact that $[P, R] = 0$, the commutation of the two C-operators is equivalent to $C^2 = C'^2 = 1$ (see theorem 5.1).

The last assertion (108) is now deduced by first noting that (44) and (89) imply that C obeys

$$C E_k = P\eta E_k = E_{N-k} C. \tag{110}$$

In other words, C corresponds to parity reversal within the Temperley–Lieb algebra, i.e. it implements the algebra automorphism $\gamma : e_k \to e_{N-k}$. A similar relation holds for the Hecke algebra generators via (17). The representation $\mathcal{B}$ of the braid β in (109) invokes the same automorphism,

$$b_j \beta = \beta b_{N-j}, \qquad 1 \leqslant j < N, \tag{111}$$

which can be verified directly on the abstract algebra level using the relation

$$b_j \beta_{j-1} \beta_j = \beta_{j-1} \beta_j b_1. \tag{112}$$

The last identity is most easily checked graphically by identifying the b_i's with the generator of Artin's braid group acting on N strings. β is also invertible, and we can conclude that $C\mathcal{B}^{-1}$ commutes with the Temperley–Lieb action. Hence, we must have

$$C\mathcal{B}^{-1}|_{\Gamma_j^{(r)}} = \chi_j$$

for some scalar $\chi_j \in \mathbb{C}$. This completes the proof. $\qquad\square$

In order to completely fix the algebraic expression for C we need to compute the missing scalar factors χ_j on each invariant subspace $\Gamma_j^{(r)}$. Due to the fact that $C^2 = 1$ the latter are simply determined by computing the value of the central element $\mathcal{B}^2$ on each $\Gamma_j^{(r)}$. In appendix B, we present this computation for q generic on the unrestricted path space Γ_j using diagrammatic techniques. Here we argue that this result extends to the root of unity case as well.

Lemma 5.1. *Let* $\beta \in H_N(q)$ *be defined as in (109). Denote by* $\varrho_j^{(r)}$ *the irreducible representation given by restricting (77) to* $\Gamma_j^{(r)}$, *i.e. all restricted paths on the Bratelli diagram ending at* j. *Then*

$$\varrho_j^{(r)}(\beta^2) = q^{-\frac{N(N-4)}{2} - 2j(j+1)} \tag{113}$$

and hence

$$\chi_j = q^{\frac{N(N-4)}{4} + j(j+1)} \tag{114}$$

in theorem 5.2.

Proof. We start from the result that $\pi_j(\beta^2) = q^{-\frac{N(N-4)}{2} - 2j(j+1)}$ for generic q on the irreducible subspace Γ_j (see appendix B for the proof). Since $\mathcal{B}^2$ remains central when taking the limit $q \to q'$ with $q' = \exp(i\pi/r)$, r integer $\geqslant 3$, it suffices to evaluate $\mathcal{B}^2$ on any path which will belong to the restricted subspace $\Gamma_j^{(r)}$. Obviously, there always exists such a path, for instance take the path j' from (101) in the proof of theorem 5.1. This fixes χ_j in (108) up to a sign. We take the same (principal) branch as used in the matrix elements (88) of η. $\qquad\square$

For illustration we state in table 3 below the powers occurring in (113) for some examples.

Table 3. Negative powers y of q occurring in the restriction $\beta^2|_{\Gamma_j} = q^{-y}$.

$N \backslash j$	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$	3	$\frac{7}{2}$	4	$\frac{9}{2}$	5
3		0		6							
4	0		4		12						
5		4		10		20					
6	6		10		18		30				
7		12		18		28		42			
8	16		20		28		40		56		
9		24		30		40		54		72	
10	30		34		42		54		70		90

5.2. The case when q is not a root of unity

Somewhat paradoxically the case when q is on the unit circle but not a root of unity is simpler from an algebraic point of view and yet the discussion of quasi-Hermiticity in terms of the path basis becomes more involved. This is due to the fact that the restriction (76) on the paths on the Bratelli diagram is lifted, and the q-integers appearing in the representation (77) can now change sign as the path progresses. Namely, parametrizing as before $q = \exp(i\pi/r)$ but now with $r \in \mathbb{R}$ we have

$$[2j + 1]_q > 0, \qquad 2\ell r < 2j + 1 < (2\ell + 1)r,$$

$$[2j + 1]_q < 0, \qquad (2\ell + 1)r < 2j + 1 < (2\ell + 2)r, \quad [2j + 1]_q > 0, \quad \ell = 0, 1, 2, \ldots. \tag{115}$$

Thus, positivity of the q-integers along a path $j \in \Gamma$ is only guaranteed as long as $r > N$. For this segment of the unit circle the previous constructions and results apply verbatim, with the exception that the Hamiltonian is diagonalizable without any restriction being placed on the state space.

6. Conclusions

In this paper, we have carried out a detailed and exact analysis of PT symmetry and quasi-Hermiticity for the quantum group symmetric XXZ spin chain. This model has two key advantages as a laboratory for the in-depth investigation of these ideas: it is finite-dimensional, and it is exactly solvable. As a consequence of the latter property, there is a well-developed and rich algebraic description of this model. We have used this algebraic machinery in order to construct an exact expression for the η operator, whose key property $\eta H = H^*\eta$ demonstrates the quasi-Hermiticity of the model for q a root of unity. In order to develop this construction, we have been inevitably led to carry out the procedure of quantum group reduction. We have thus constructed η, given by equation (87), in terms of the path basis in which this reduction is well defined. Moreover, this construction linked the question of determining whether H is quasi-Hermitian to the mathematical problem of finding a self-adjoint representation of the Temperley–Lieb algebra.

Bender and others have introduced the idea of a C operator in the discussion of PT symmetry [6] which is closely connected with the notion of quasi-Hermiticity [9]. We too have defined such a C operator as $C = P\eta$ (P is the parity operator as discussed in the main text). This operator is very natural from an algebraic point of view, and has the realization in terms of the braid β given by (108).

Table 4. Commutation relations for the operator η and the two *C*-operators.

Operator	Hamiltonian	Temperley–Lieb	Quantum group
η	$\eta H = H^* \eta$	$\eta E_k = E_k^* \eta$	$\eta S^{\pm} = S_{\mathrm{op}}^{\pm} \eta$
$C = P\eta$	$[C, H] = 0$	$C E_k = E_{N-k} C$	$[C, S^{\pm}] = [C, S^z] = 0$
$C' = R\eta$	$[C', H] = 0$	$[C', E_k] = 0$	$C' S^{\pm} = S^{\mp} C', \ C' S^z = -S^z C'$

Two algebras appear in the description of the quantum spin chain: the quantum group and the Temperley–Lieb. The quantum version of Schur–Weyl duality tells us that each is the commutant of the other. The algebraic construction of C combined with this duality led us naturally to define a new operator $C' = R\eta$ (here R is the spin-reversal operator) with similar but dual properties to C and with $[C', C] = 0$. These properties are summarized in table 4.

We have given a construction of η, and thus a proof of the reality of the spectrum of (7), that is valid for $q = \exp(\mathrm{i}\pi/r)$ for two regions: r an integer $\geqslant 3$; and $r > N$ (see section 5.2). It is commonly assumed that the spectrum of the model is also real for q on the unit circle outside this region (see, e.g., [14]). To the best of our knowledge this assumption is based on numerical investigations of the Bethe ansatz equations and a rigorous proof of this assertion is missing. (Obviously, the spectrum is also real when $q \in \mathbb{R}$, for which the Hamiltonian is Hermitian with respect to the original canonical inner product on $V^{\otimes N}$.) Clear questions remain as to whether the model is also quasi-Hermitian in this region, whether there is a clear criterion that shows this, and if so, whether there is a simple alternative construction of η. Preliminary numerical tests which we have carried out seem to indicate that one in general has to drop the more stringent condition that η intertwines the Temperley–Lieb generators, i.e. $\eta E_k = E_k^* \eta$.

Finally, we point out that we have also omitted the case $r = 2$ or $q = \sqrt{-1}$ from our discussion as this case is rather special. The quantum group reduction as discussed here does not apply to this case and the corresponding question of quasi-Hermiticity will be investigated in a separate publication [27].

Acknowledgments

Appendix A. Kauffman diagrams and Levy's reduced words

In this appendix we review briefly the known graphical calculus associated with the Temperley–Lieb algebra and give a characterization of its irreducible representations which is slightly different from that in the main text. We then will employ this graphical calculus in appendix B to compute the values of the central element β^2 defined in equation (109) of theorem 5.2.

We follow ideas put forward by Kauffman [28], and we adopt the conventions of [29] to describe the irreducible representations of $TL_N(q)$ using primitive left ideals of the Temperley–Lieb algebra. In what follows we let q be generic, i.e. we treat q as a formal indeterminate.

Definition A.1 (Levy [29]). *A word $w = e_{i_1} e_{i_2} \cdots e_{i_n} \in TL_N(q)$ in the Temperley–Lieb generators is said to possess a 'jump' if the indices of two neighbouring generators differ by more than one, i.e. $|i_k - i_{k+1}| > 1$ for some $k = 1, \ldots, n-1$.*

Obviously, the maximum value $k_{\max}$ of jumps which can occur in a word w is $k_{\max} = \lfloor N/2 \rfloor - 1$, where $\lfloor N/2 \rfloor$ is the integer part of $N/2$.

Definition A.2 (Levy). *Let $I_k \subset TL_N(q)$ be the left primitive ideal consisting of all words having at least k jumps. Setting $I_{-1} \equiv TL_N(q)$ we define for each $-1 < k < k_{\max}$ the (vector space) quotient*

$$W_k = I_k / I_{k+1}, \tag{A.1}$$

i.e. the set of all words which have precisely k jumps. For $k = -1$ we have $W_{-1} = \mathbb{C}$ and for $k = k_{\max}$ we set $W_{k_{\max}} = I_{k_{\max}}$.

Regarded as a vector space, W_k is equipped with a natural action of $TL_N(q)$ and gives rise to an irreducible representation,

$$\rho_k : TL_N(q) \to \operatorname{End} W_k, \quad a \mapsto \rho_k(a) \qquad \text{with} \quad \rho_k(a)w := aw. \tag{A.2}$$

In order to identify the representations ρ_k with the correct path representation ϱ_j over Γ_j given in the main text—see (77) and (80)—we need to compare dimensions. To this end we follow Levy and introduce for each W_k a basis in terms of the reduced words

$$w_n^{(m)} = e_m e_{m-1} \cdots e_n, \qquad m > n \tag{A.3}$$

defining the basis elements to be

$$w_{m_1, \ldots, m_{k+1}} = w_1^{(m_1)} w_3^{(m_2)} \cdots w_{2k+1}^{(m_{k+1})}, \qquad 1 \leqslant m_1 < \cdots < m_{k+1} \leqslant N-1, \qquad m_i > 2i - 1. \tag{A.4}$$

From this basis definition, one computes the corresponding dimensions to be

$$\dim W_k = \binom{N-1}{k+1} - \binom{N-1}{k-1}. \tag{A.5}$$

Upon comparing this result with the multiplicity formula (82) on the Bratelli diagram one can conclude that the following representations are isomorphic:

$$W_k \cong \Gamma_{j=N/2-k-1}. \tag{A.6}$$

Our motivation for introducing the representations ρ_k is that they allow for a convenient graphical calculus. For given k, each basis element in (A.4) corresponds to a diagram of $k+1$ (possibly nested) caps and $N - 2(k+1)$ vertical lines on which the Temperley–Lieb generators e_i act in a simple manner. We demonstrate this for a simple example to keep this paper self-contained.

A.1. Example $N = 6$

Let the identity element in $TL_N(q)$ correspond to a diagram consisting of $N = 6$ strands and each Temperley–Lieb generator e_k be represented by a diagram similar to that for e_3 depicted in the figure below,

$$\tag{A.7}$$

The algebra multiplication corresponds to composing diagrams from below. The basis elements (A.4) spanning W_k should be considered as equivalence classes of words. By

abuse of notation we denote them by the same symbols as the algebra elements. Since I_k is a left ideal and the algebra action in (A.2) is defined to be from the left it suffices to depict the elements (A.4) by the bottom half of their respective diagrams. For instance for $N = 6$ and $k = k_{\max} = 2$ we have the five words

$$e_1 e_3 e_5 = \frown\ \frown\ \frown \quad , \qquad e_1\ e_4 e_3\ e_5 = \frown\ \overset{\frown}{\frown}\ , \tag{A.8}$$

$$e_2 e_1\ e_3\ e_5 = \overset{\frown}{\frown}\ \frown\ , \qquad e_2 e_1\ e_4 e_3\ e_5 = \overset{\frown}{\frown\ \frown}\ , \tag{A.9}$$

and

$$e_3 e_2 e_1\ e_4 e_3\ e_5 = \overset{\overset{\frown}{\frown}}{}\ . \tag{A.10}$$

The action of the Temperley–Lieb algebra on these five diagrams from below leads to simple permutations of the basis elements. For example acting with e_2 on the first diagram we obtain

$$\text{(diagram)} = \text{(diagram)}\ . \tag{A.11}$$

Any closed loops occurring in this process yield factors $-(q + q^{-1})$ according to the defining relation $e_i^2 = -(q + q^{-1})e_i$.

Appendix B. Computation of β^2

We now turn to the graphical computation of the central element $\beta^2 \in H_N(q)$ involving the braid β defined in (109). The Hecke algebra generators also have a graphical representation. Namely, each generator b_i acts on the identity diagram of N parallel strands by crossing the ith strand over the $(i + 1)$th one. For b_i^{-1} the $(i + 1)$th strand is on top. The braid β has then the following graphical depiction,

$$\beta = \qquad \tag{B.1}$$

where the NW-SE lines cross over the NE-SW lines. In order to compute the action of β^2 on the basis elements in $W_k \cong \Gamma_{j=N/2-k-1}$ we need further graphical rules. All of them are a direct consequence of the homomorphism (17) which graphically amounts to the following equality of diagrams,

$$\times = q^{-1}\ \Big|\ \Big| + \underset{\frown}{\smile} \tag{B.2}$$

An analogous picture holds for the relation $b_i^{-1} \to q + e_i$. Repeated use of these relations together with the defining relations of the Temperley–Lieb generators now yields the following

Lemma B.1. *Employing identification (17) one verifies the following identities*

- $b_i e_i = -q e_i$; *compare with the depiction below.*

$$\tag{B.3}$$

- $b_i b_{i\pm 1} e_i = q^{-1} e_{i\pm 1} e_i$; *see the pictures below.*

$$\tag{B.4}$$

Proof. A trivial computation follows either directly from the identification (17), or from the graphical rule (B.2) together with the identification of a complete circle with the coefficient $-(q + q^{-1})$. □

We are now in a position to derive the values of the central element β^2 in the irreducible representation (77) over the path space Γ_j.

Lemma B.2. *Assume q to be generic and let $\beta \in H_N(q)$ be defined as in (109), i.e.*

$$\beta = \beta_1 \beta_2 \cdots \beta_{N-1}, \qquad \beta_n = b_n b_{n-1} \cdots b_1.$$

Denote by ϱ_j the irreducible representation given by (17) and restricting (77) to Γ_j, i.e. all paths on the Bratelli diagram ending at j. Then

$$\varrho_j(\beta^2) = q^{-\frac{N(N-4)}{2} - 2j(j+1)}. \tag{B.5}$$

Proof. According to our remarks in appendix A we can exploit the fact that for generic q the finite-dimensional irreducible representations of $TL_N(q)$ respectively $H_N(q)$ are determined by their dimensions up to isomorphism. Since β^2 is central, its value does not depend on the particular choice of the representation as long as we stay in the same isomorphism class. We can therefore identify $W_k \cong \Gamma_{j=N/2-k-1}$ and compute the action of β on the reduced words in W_k, where it is particularly simple. According to Schur's lemma it does not matter which word we use and we focus our attention on the word $w_{1,3,5,\ldots,2k+1}$ depicted below,

$$\tag{B.6}$$

Acting with β on this word from below we obtain the diagram shown here

$$(B.7)$$

We will now undo this braid in a number of successive steps using the diagrammatic rules of the preceding lemma. We start with the left most cap. Employing rule (i) of the preceding lemma we untwist it once and obtain a factor $-q$. Applying rule (ii) from the previous lemma we pull it over $N-2$ NE-SW lines producing the factor $-q^{3-N}$. The resulting diagram is depicted below.
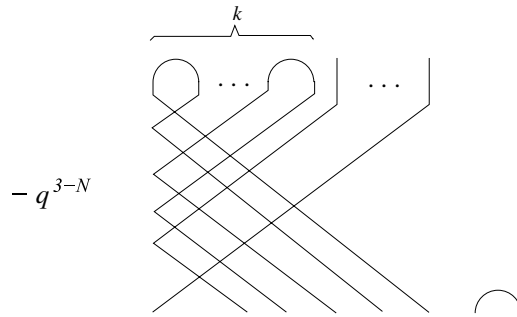
$$-q^{3-N} \qquad (B.8)$$

Thus, we are back at the starting point, but now with a diagram which has one less cap. Repeating the same steps as before we end up with the diagram
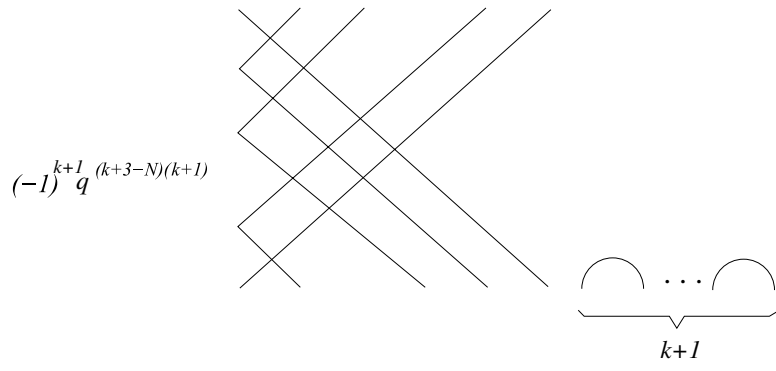
$$(-1)^{k+1} q^{(k+3-N)(k+1)} \qquad (B.9)$$

from which all caps are removed. In the remaining graph we need to undo all the crossings of lines according to (B.2). However, we can discard all the terms which introduce additional caps since according to (A.1) these are identified with zero under the quotient. Thus, each of

the $(N - 2k - 3)(N - 2k - 2)/2$ vertices in the diagram (B.9) yields a factor q^{-1} and we end up with the diagram

$$(-1)^{k+1}q^{-N(N-2k+3)/2-k(k+1)} \qquad | \quad \dots \quad | \qquad \frown \quad \dots \quad \frown$$

(B.10)

Up to a factor, we have simply obtained the diagram reflected about the vertical axis. By reflection symmetry we deduce that applying β twice simply produces the q-factor in (B.10) to the power two. Upon replacing $k + 1 = N/2 - j$ according to (A.6) we obtain the desired result. □

Appendix C. Derivation of the Clebsch–Gordan coefficients

In this section, we derive the Clebsch–Gordan coefficients (71), (72) entering the definition of the path basis vectors (74) according to (75). We use the convention (69) for the irreducible representations of the quantum group $U_q(sl_2)$. We include these details as some derivations in the literature are known to contain minor errors.

C.1. The CG coefficients for $J = j + 1/2$, $j_1 = j$, $j_2 = 1/2$

We start with the representation $\pi_{j+1/2} \subset \pi_j \otimes \pi_{1/2}$ and take as a highest weight vector

$$|J, M = J\rangle = |j, j\rangle \otimes \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle.$$

(C.1)

Successive action with $\Delta(S^-)$ on the highest weight vector yields the expression

$$\Delta(S^-)^m |J, J\rangle = q^{j - \frac{m-1}{2}} [m] \left(\frac{[2j]![m-1]!}{[2j-m+1]!}\right)^{\frac{1}{2}} |j, j - m + 1\rangle \otimes \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle$$

$$+ q^{-\frac{m}{2}} \left(\frac{[2j]![m]!}{[2j-m]!}\right)^{\frac{1}{2}} |j, j - m\rangle \otimes \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle$$

$$= \left(\frac{[2J]![m]!}{[2J-m]!}\right)^{\frac{1}{2}} |J, J - m\rangle = \left(\frac{[2j+1]![m]!}{[2j-m+1]!}\right)^{\frac{1}{2}} |J, J - m\rangle.$$

(C.2)

From this formula we infer the first identity (71) for the CG coefficients.

C.2. The CG coefficients for $J = j - 1/2$, $j_1 = j$, $j_2 = 1/2$

We now turn to the representation $\pi_{j-1/2} \subset \pi_j \otimes \pi_{1/2}$. The highest weight vector is now determined by the relation (the factor $q^{-1/2}$ is introduced to obtain a more symmetric expression for the CG coefficients)

$$0 = \Delta(S^+) |J, J\rangle = \Delta(S^+)\left\{q^{-\frac{1}{2}}|j, j\rangle \otimes \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle + \gamma q^{-\frac{1}{2}}|j, j - 1\rangle \otimes \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle\right\}$$

(C.3)

and one easily finds

$$\gamma = -\frac{q^{j+\frac{1}{2}}}{[2j]^{\frac{1}{2}}}.$$

(C.4)

In a similar manner as above, one proves by induction that

$$\Delta(S^-)^m|J,J\rangle = q^{-\frac{m+1}{2}}[2j-m]\left(\frac{[2j-1]![m]!}{[2j][2j-m]!}\right)^{\frac{1}{2}}|j,j-m\rangle\otimes\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle$$

$$- q^{j-\frac{m}{2}}\left(\frac{[2j-1]![m+1]!}{[2j][2j-m-1]!}\right)^{\frac{1}{2}}|j,j-m-1\rangle\otimes\left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle$$

$$= \left(\frac{[2J]![m]!}{[2J-m]!}\right)^{\frac{1}{2}}|J,J-m\rangle = \left(\frac{[2j-1]![m]!}{[2j-m-1]!}\right)^{\frac{1}{2}}|J,J-m\rangle. \qquad (C.5)$$

From this result we read off

$$\begin{vmatrix} j & \tfrac{1}{2} & j-\tfrac{1}{2} \\ m & \alpha & m+\alpha \end{vmatrix}_q = -2\alpha q^{\alpha(j+1)+\frac{m}{2}}\left(\frac{[j-2\alpha m]}{[2j]}\right)^{\frac{1}{2}}. \qquad (C.6)$$

In order to have the crucial identity

$$\sum_{m,\alpha}\begin{vmatrix} j & \tfrac{1}{2} & j' \\ m & \alpha & m' \end{vmatrix}_q\begin{vmatrix} j & \tfrac{1}{2} & j'' \\ m & \alpha & m'' \end{vmatrix}_q = \delta_{j',j''}\delta_{m',m''} \qquad (C.7)$$

we renormalize the CG coefficients by the factor $-\sqrt{[2j+1]/[2j]}$ such that we obtain the second identity (72).

C.3. Identities involving the CG coefficients

For the derivation of (77) one requires the following set of identities, which we list without proof.

$$\begin{vmatrix} j\pm\tfrac{1}{2} & \tfrac{1}{2} & j \\ m+\alpha & -\alpha & m \end{vmatrix}_q = \mp 2\alpha q^{-\alpha}\sqrt{\frac{[2j+1]}{[2j+1\pm1]}}\begin{vmatrix} j & \tfrac{1}{2} & j\pm\tfrac{1}{2} \\ m & \alpha & m+\alpha \end{vmatrix}_q$$

$$\begin{vmatrix} j & \tfrac{1}{2} & j\pm\tfrac{1}{2} \\ m & \alpha & m+\alpha \end{vmatrix}_q\begin{vmatrix} j\pm\tfrac{1}{2} & \tfrac{1}{2} & j\pm1 \\ m+\alpha & -\alpha & m \end{vmatrix}_q = q^{2\alpha}\begin{vmatrix} j & \tfrac{1}{2} & j\pm\tfrac{1}{2} \\ m & -\alpha & m-\alpha \end{vmatrix}_q\begin{vmatrix} j\pm\tfrac{1}{2} & \tfrac{1}{2} & j\pm1 \\ m-\alpha & \alpha & m \end{vmatrix}_q$$

$$\begin{vmatrix} j & \tfrac{1}{2} & j\pm\tfrac{1}{2} \\ m & \alpha & m+\alpha \end{vmatrix}_q\begin{vmatrix} j\pm\tfrac{1}{2} & \tfrac{1}{2} & j \\ m+\alpha & -\alpha & m \end{vmatrix}_q$$

$$= -q^{-2\alpha(2j+1)}\frac{\left[j\pm2\alpha m+\frac{1\pm1}{2}\right]}{\left[j\mp2\alpha m+\frac{1\pm1}{2}\right]}\begin{vmatrix} j & \tfrac{1}{2} & j\pm\tfrac{1}{2} \\ m & -\alpha & m-\alpha \end{vmatrix}_q\begin{vmatrix} j\pm\tfrac{1}{2} & \tfrac{1}{2} & j \\ m-\alpha & \alpha & m \end{vmatrix}_q$$

$$\sum_{j'=j\pm1/2}[2j'+1]^{\frac{1}{2}}\begin{vmatrix} j & \tfrac{1}{2} & j' \\ m & \alpha & m+\alpha \end{vmatrix}_q\begin{vmatrix} j' & \tfrac{1}{2} & j \\ m+\alpha & \alpha & m+2\alpha \end{vmatrix}_q = 0$$

$$\sum_{j'=j\pm1/2}\pm[2j'+1]^{\frac{1}{2}}\begin{vmatrix} j & \tfrac{1}{2} & j' \\ m & \alpha & m+\alpha \end{vmatrix}_q\begin{vmatrix} j' & \tfrac{1}{2} & j \\ m+\alpha & -\alpha & m \end{vmatrix}_q = -2\alpha q^{-\alpha}[2j+1]^{\frac{1}{2}}$$

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