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On the Spectrum of the XXZ-Chain at Roots of Unity

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In a recent paper (cond-mat/0009279), Fabricius and McCoy studied the spectrum of the spin 1/2 XXZ model at roots of unity, i.e., $\Delta=(q+q^{-1})/2$ with $q^{2N}=1$ for integer $N\geqslant 2$. They found a certain pattern of degeneracies and linked it to the sl_2-loop symmetry present in the commensurable spin sector—$S^z\equiv 0 \bmod N$. We show that the degeneracies are due to an unusual type of zero-energy "transparent" excitation, the *cyclic bound state*. The cyclic bound states exist both in the commensurable and in the incommensurable sectors indicating a symmetry group present, of which sl_2-loop algebra is a partial manifestation. Our approach treats both sectors on even footing and allows us to obtain analytically an explicit expression for the degeneracies in the case $N=3$.

KEY WORDS: Integrable models; quantum symmetry; spin chains; multiplets; elementary excitations.

1. INTRODUCTION

In a recent interesting work[1,2] the spin-1/2 XXZ model,

$$H=\sum_{j=1}^{L} \sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+ + (\Delta/2)\,\sigma_j^z\sigma_{j+1}^z, \tag{1}$$

was studied on a chain with L sites and periodic boundary conditions ($\sigma_{L+1}=\sigma_1$) for the special values of the anisotropy.

$$\Delta=\tfrac{1}{2}(q+q^{-1}) \qquad \text{with} \quad q^{2N}=1, \tag{2}$$

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A large symmetry algebra was shown to be present, manifesting itself in a rich pattern of degeneracies.

For $N=2$, $\Delta=0$ the study was carried out analytically. The model reduces to the XY model, equivalent to free fermions. The degeneracies, in this case, are due to "pairs" of spin-down excitations with momenta $p_{1,2}$, satisfying the condition

$$p_1+p_2=\pi \bmod 2\pi,$$

because the energy of the "pair" is zero:

$$\cos p_1+\cos p_2=0.$$

A combinatorial argument[1] then shows that an eigenstate with $S^z=S^z_{\max}$ is degenerate with states having different spin $S^z=S^z_{\max}-2l$, $0\leqslant l\leqslant S^z_{\max}$. The dimension of the multiplet with $S^z=S^z_{\max}-2l$ is (assuming L to be even):

$$\binom{S^z_{\max}}{l}, \tag{3}$$

if $S^z_{\max}$ is even, otherwise it is

$$\binom{S^z_{\max}\pm 1}{l}, \tag{4}$$

with the $(\pm)$-sign depending on the $S^z_{\max}$ "parent state." Whereas the formula, Eq. (3), for the commensurable case (2 divides $S^z_{\max}$), is independent of the parent state, the formula for the incommensurable case, Eq. (4), although similar, does depend on it.

Deguchi *et al.*[1] relate this degeneracy to the sl_2-loop algebra, which is a symmetry of the Hamiltonian for $\Delta=0$ and $S^z_{\max}$ even. This symmetry is not realized in the case $S^z_{\max}$ odd, but in ref. 1 it is argued that a certain residual of it is still responsible for the degeneracies given by (4).

The degeneracies for $N\geqslant 3$ were studied numerically in ref. 1 and the authors found a surprisingly simple generalization of (3), (4): The state with $S^z=S^z_{\max}$ is degenerate with states having $S^z=S^z_{\max}-lN$, and the corresponding multiplet has dimension,

$$\binom{2S^z_{\max}/N}{l} \tag{5}$$

in the commensurable case,

$$S^z_{\max}\equiv 0 \bmod N, \tag{6}$$

and

$$\binom{2[S^z_{\max}/N]+\alpha}{l} \tag{7}$$

in the incommensurable case, N does not divide $S^z_{\max}$ ($[x]$ is the Gauss step function and α may take values 0, 1, or 2).

In this paper we show that the degeneracies arise due to the presence of multi-particle *transparent* excitations which are present in the spectrum for q at a root of unity. Transparent excitations are spin carrying, zero-energy excitations that can be added to an eigenstate, without changing its Bethe–Ansatz parameters, leading this way to degenerate multiplets, manifestation of some underlying symmetry. As this symmetry patterns are present in the full Hilbert space the symmetry cannot be identified with the $sl(2)$-loop, valid only in commensurable sectors. Our approach allows us to derive an analytic expression for the multiplet degeneracies and, in particular in the incommensurable case, identify what feature of the parent state leads to the various degeneracies.

Our paper is organized as follows. In Section 2 we discuss the $SU(2)$ and quantum group $U_q(sl_2)$ symmetries in the spin-1/2 chains and give an interpretation of these symmetries within the Bethe ansatz language in terms of single-particle *transparent* excitations.

In Section 3 we introduce a class of multi-particle *transparent* excitations. They are allowed only when the anisotropy of the XXZ-chain has property (2), and lead to the multiplets described by (5) and (7). We give the general construction and properties of these states for all N. Then we specialize to the simplest nontrivial case $N=3$ and derive formula (5) for $l=1$ while giving an argument for its validity for $l>1$. In the incommensurable case we show that three cases arise when the degeneracy of a multiplet built on a $S^z_{\max}$ parent state is considered, these cases corresponding to the presence in it of the special single-particle excitations, considered in Section 2.

The concluding section gives some numerical examples, which indicate that most but not all degeneracies of the spectrum can be explained within this framework. The appendix provides technical details.

2. TRANSPARENT EXCITATIONS AND SYMMETRIES OF THE SPIN CHAIN

A spin state in the sector with fixed $S^z \geqslant 0$ can be written as,

$$|\Psi\rangle = \sum_{1\leqslant n_1<\cdots n_M\leqslant L} f(n_1,\ldots,n_M)\,\sigma^-_{n_1}\cdots\sigma^-_{n_M}\,|0\rangle, \tag{8}$$

with $M = L/2 - S^z$ and the reference state $|0\rangle$ having all spins up. For eigenstates of (1) the coefficients $f(n_1, \ldots, n_M)$ take a Bethe ansatz form:

$$f(n_1, \ldots, n_M) = \sum_{P \in S_M} A_P \exp\left(i \sum_j^M k_{P(j)} n_j \right), \tag{9}$$

parameterized by M numbers, the spin momenta k_j, $j = 1 \cdots M$. Imposing periodic boundary conditions the k_j are determined by:

$$e^{-ik_j L} = \prod_{l \neq j}^{M} S(k_j, k_l), \tag{10}$$

where the S-matrices $S(k_j, k_l)$ are:

$$S(k_j, k_l) = -\frac{e^{i(k_j + k_l)} + 1 - 2\Delta e^{ik_l}}{e^{i(k_j + k_l)} + 1 - 2\Delta e^{ik_j}}. \tag{11}$$

The $S(k_j, k_l)$ are determined from (1) and relate the amplitude in the wave function for the down-spin (magnon) associated with k_j to be to the left of the magnon associated with k_l, to the amplitude with their order reversed.

Introducing the λ-parameterization via,

$$e^{ik_j} = -\frac{\sinh \frac{\gamma}{2} (\lambda_j + i)}{\sinh \frac{\gamma}{2} (\lambda_j - i)} \tag{12}$$

with γ defined by $\Delta = (q + q^{-1})/2 = -\cos \gamma$, $-1 < \Delta < 1$, the S-matrices take the form,

$$S(\lambda_j - \lambda_k) = \frac{\sinh \frac{\gamma}{2} (\lambda_j - \lambda_k - 2i)}{\sinh \frac{\gamma}{2} (\lambda_j - \lambda_k + 2i)}. \tag{13}$$

For the case $\Delta = 1$, the XXX model, we have instead

$$e^{ik_j} = \frac{\lambda_j + i}{\lambda_j - i} \tag{14}$$

and

$$S(\lambda_j - \lambda_k) = \frac{\lambda_j - \lambda_k - 2i}{\lambda_j - \lambda_k + 2i}. \tag{15}$$

Having characterized the states we proceed to study the manifestations of symmetry in the spectrum, relating it to the presence of *transparent* excitations—a concept which we shall significantly generalize as we progress. Begin with the XXX-chain ($\Delta = 1$) which is $SU(2)$ invariant. The BA equations (10) determine the parameters $\lambda_1,\dots,\lambda_M$ under the assumption that all of them are finite. What happens, if some of the λ diverge? For $\lambda_0 \to \infty$, the S-matrix (15), $S(\lambda_0, \lambda_k) \to 1$, independently of λ_k, and the corresponding factors drop out of (10). That means, given a set of finite $\lambda_1 \cdots \lambda_M$, which describe an eigenstate with $S^z_{\max} = L/2 - M$, one can generate an eigenstate with $S^z = S^z_{\max} - l$ by adding l spin down excitations with parameter $\lambda = \infty$. The physical interpretation of these "singular" values of the λ's is very simple: They are nothing but elementary excitations ("magnons") with momentum $k_0 = 0$ and energy $E = 0$. These states have S-matrix $S(0, k_j) = 1$ with all other particles and among themselves, they are therefore *transparent*, which is the reason that more than one of them can appear in an eigenstate of (1). (For nonzero k_j, the S-matrix $S(k_j, k_j) = -1$, forbidding more than one excitation having momentum k_j). By "adding" we mean the following operation: Given the amplitudes A_P in (9) we construct the components of the wavefunction $f(n_1,\dots, n_M, n_{M+1},\dots, n_{M+l})$ through,

$$f(n_1,\dots, n_M, n_{M+1},\dots, n_{M+l}) = \sum_{Q \in S_{M+l}} A_{P(Q)} \exp\left(i \sum_j^{M+l} k_{Q(j)} n_j\right). \tag{16}$$

Here $P(Q)$ denotes a permutation $\in S_M$, such that for $1 \leqslant j \leqslant M$:

$$P^{-1}(j) = \text{number of } m \in \{1 \cdots M\} \qquad \text{for which} \quad Q^{-1}(m) \leqslant Q^{-1}(j). \tag{17}$$

and $k_l = 0$ for $l > M$. (An example of the construction is given in Appendix A.1.) This way we may construct the explicit Bethe wavefunction of a state containing l of the zero-momentum excitations, given an eigenstate (8) of the hamiltonian described by momenta $\{k_j\}$ and amplitudes $\{A_P\}$.

The new states can be generated directly from the state (8) by acting on it l times with the operator

$$\hat{S}^- = \sum_{j=1}^{L} \sigma_j^-, \tag{18}$$

which coincides with the spin lowering operator in the L-fold product of spin $1/2$ representations. The global $SU(2)$ symmetry corresponds therefore to the existence of transparent excitations with zero energy. At the same time, this leads to singular parameters in the Bethe ansatz.

Now examine the case $\Delta \neq 1$, i.e., $q \neq 1$. Here the situation is more interesting. Introducing k_q via $e^{ik_q} = q$, we note that the momentum k_q particle has zero energy and interacts (see Eq. (11)) with other particles k_j via an S-matrix,

$$S(\pm k_q, k_j) = q^{\mp 2}, \tag{19}$$

that is independent of k_j. However $S(\pm k_q, k_j) \neq 1$, so this excitation is *not* transparent. The independence of the S-matrix on the momentum k_j of the second particle makes the excitation with $\pm k_q$ nevertheless a candidate for a quantum symmetry, which would operate on a state without affecting the parameters $\{k_j\}$ of that state as in (16). Moreover, as numerator and denominator of $S(k_q, k_q)$ vanish, the S-matrix of these states among themselves can be chosen to be unity and therefore more than one of them can appear in a given state. This is not the case for periodic BC where the parameters $\{k_j\}$ of the parent state are affected by adding l excitations with $\pm k_q$. The Bethe–Ansatz equation now are:

$$e^{-ik_jL} = \prod_{l \neq j}^{M} S(k_j, k_l)\, q^{\pm 2l} \tag{20}$$

$$q^{\pm L} = q^{\pm 2M}, \tag{21}$$

and not only lead to a shift of the parameters k_j of the parent state but they are consistent only at special values of $S^z = L/2 - M$ and q: $q^{L-2M} = 1$. Therefore the XXZ model with periodic BC does not possess this symmetry in general.[3]

However under certain conditions, the states with $\pm k_q$, can exist on a periodic chain. Assume that $q^{2N} = 1$. Then adding mN, $m = 1, 2,\ldots$ excitations with momentum k_q leaves the original equations unmodified (Eq. (20) coincides with (10)), because the N particles *together* are again transparent. But we have still equation (21), which entails that

$$S^z \equiv 0 \bmod N. \tag{22}$$

[3] The k_j are shifted by a constant, this is equivalent to a boundary twist. Adding a boundary term[6] to the hamiltonian with open BC, the excitation with k_q becomes allowed: The boundary field is constructed in a way that this state (but not the state with $-k_q$!) is not reflected at the boundary and therefore we do not have (21). Moreover, in the open boundary equation analogous to (20), the q-dependent factor drops out and the parameters of the parent state are unchanged. The $U_q(sl_2)$ symmetry is then manifest.

That means, that in certain sectors of the Hilbert space, satisfying the commensurability condition (22), the excitation containing N of the elementary ones has zero energy and is transparent to all other excitations. Together with other transparent excitations, to be discussed in the next section, it induces a quantum symmetry (that means, it has no classical counterpart as for the XXX-chain).

In terms of the λ_j-parameterization, the k_q-state is again singular: $\lambda_q = \infty$, rendering this parameterization useless in dealing with the q-symmetry. The formula for $f(n_1,..., n_{M+1})$ is now more complicated than (16), because $k_q \neq 0$ and the S-matrices (19) are nontrivial. Nevertheless the state can be constructed, because its BA equations are the same as for the parent state. Further, there is an analogue to (18), namely,

$$\hat{S}_q^- = \sum_{j=1}^{L} q^{\sigma^z/2} \otimes \cdots \otimes \sigma_j^- \otimes \cdots \otimes q^{-\sigma^z/2}, \tag{23}$$

which is the quantum deformed version of the spin lowering operator, belonging to $U_q(sl_2)$. The noncommutative coproduct structure of $U_q(sl_2)$ is just well suited to generate the wavefunction having an excitation with k_q in accord with $S(k_q, k_j) = q^{-2}$. The isomorphic representation,[7]

$$\hat{T}_q^- = \sum_{j=1}^{L} q^{-\sigma^z/2} \otimes \cdots \otimes \sigma_j^- \otimes \cdots \otimes q^{\sigma^z/2}, \tag{24}$$

likewise creates a state with $-k_q$.

While these are not symmetry operations, we saw that exciting N k_q s or $-k_q$ s does induce symmetry. The generators for both of these are,

$$S^{-(N)} = \frac{(\hat{S}_q^-)^N}{[N]_q!}, T^{-(N)} = \frac{(\hat{T}_q^-)^N}{[N]_q!} \tag{25}$$

as follows from Eqs. (23) and (24).

In ref. 1 it was shown that $S^{\pm(N)}, T^{\pm(N)}$ together with S^z generate the sl_2-loop algebra, which is therefore a symmetry in the commensurable sectors of the periodic XXZ model at $q^{2N} = 1$. However, the incommensurable sectors do *not* have this symmetry because the excitations with $\pm k_q$ violate the periodic BC.[1]

In the following section we shall show that the excitations generated by $S^{-(N)}, T^{-(N)}$ form part of a larger set of transparent multi-particle excitations, the *cyclic bound states*, existing in the XXZ model at roots of unity. Taking all of them into account, we can derive (5) and find analogous formulae in the incommensurable case where N does not divide $S^z_{\max}$.

3. BOUND STATES AND CYCLIC BOUND STATES

In this section we show there exists a large class of transparent excitations both in the commensurable *and* in the incommensurable sectors which cannot therefore be associated with the sl_2-loop algebra indicating that the model possesses a symmetry in the full Hilbert space which in the commensurable sector will reduce to the sl_2-loop algebra.

The BA equations (10) make the implicit assumption, that none of the factors $S(k_j, k_l)$ becomes singular or 1. The modulus of some of the $S(k_j, k_l)$ may deviate from 1, corresponding to complex momenta, but none is allowed to vanish as long as L is finite.

This is not the case on the *infinite* line, where an S-matrix can vanish (or diverge) signifying a bound state. Consider eigenstates of the hamiltonian of the form $(n_1 < n_2)$:

$$f(n_1, n_2) = A_{12} e^{i(p-i\xi) n_1} e^{i(p+i\xi) n_2} + A_{21} e^{i(p+i\xi) n_1} e^{i(p-i\xi) n_2}. \tag{26}$$

Here $\xi = \ln(\cos p/\Delta)$ so that $S(p-i\xi, p+i\xi) = 0$ rendering this wavefunction normalizable—$A_{21} = 0$. Equivalently, $S(p+i\xi, p-i\xi)$ diverges. This state is therefore a bound state of two "magnons" above the ferromagnetic reference state $|0\rangle$. There exist in general bound states with an arbitrary number N of magnons in the infinite system, parameterized by complex momenta $k_1,..., k_N$ and the property that

$$S(k_j, k_{j+1}) = 0, \qquad j = 1,..., N-1. \tag{27}$$

In the finite system, these states are replaced by the so-called string solutions of (10). The momenta k_j belonging to a string do not satisfy (27), (as all S-matrices must be nonzero for finite L) but may approach zero like e^{-L}, as L goes to infinity for fixed M.

One would conclude that for finite L the singular case $S(k_j, k_l) = 0$ can never happen for any two of the parameters in the Bethe wavefunction (9).[4] We will show, however, that for $q^{2N} = 1$ and $N \geqslant 3$ there exist excitations composed of N spin down magnons satisfying,

$$S(k_j, k_{j+1}) = 0, \qquad j = 1,..., N \qquad k_{N+1} = k_1. \tag{28}$$

[4] Indeed, for a state with only two down spins like (26), the amplitude A_{21} can not be zero on a finite ring, because in this case the region $n_1 < n_2$ can not be distinguished from $n_2 < n_1$. If $S(k_1, k_2)$ vanishes, $S(k_2, k_1)$ has to be zero as well, which is impossible because $S(k_1, k_2) = S(k_2, k_1)^{-1}$. This case corresponds to $N = 2$ $(\Delta = 0)$ treated in ref. 1. The "pairs" of spin-down excitations are of course not bound states as the interaction is zero.

Such states we shall call *cyclic bound states* (cbs), because of the similarity between (27) and (28). In contrast to the ordinary bound states with property (27), they exist on a *finite* ring of length L. The reason is, that all the N "particles" making up the bound state can not penetrate each other ($S(k_j, k_{j+1}) = 0$) so that the amplitudes A_P are nonzero only for the N cyclic permutations of $1, 2,\ldots, N$. These states can not be obtained from the Bethe equations (10), because the equation determining a momentum k_j belonging to this state would contain the factor $S(k_j, k_{j+1})\, S(k_j, k_{j-1})$, i.e., the product of zero and infinity, rendering it meaningless. These states have the Bethe ansatz form (9), but their parameters are *not* given by a solution to (10).[5]

The physical interpretation of the corresponding eigenvectors is quite clear: they are a special type of bound states existing in a finite system, in contrast to the usual situation.

We see that the Bethe ansatz is, strictly speaking, more general than the Bethe ansatz equations (10): It is impossible to interpret the cbs as some "singular" type of solution to (10) as in the $SU(2)$ or $U_q(sl_2)$ case, because it will turn out that it contains a free parameter, not determined by any equation.

We demonstrate now, that for a cbs with N members to exist we must have $q^{2N} = 1$, or, in the parameterization (13),

$$\gamma = m_\gamma \frac{\pi}{N}, \qquad 1 \leqslant m_\gamma \leqslant N-1. \tag{29}$$

Using (11) and notation $x_j = e^{ik_j}$, the cbs-condition (28) reads

$$\begin{aligned} x_1 + x_2^{-1} &= 2\Delta \\ x_2 + x_3^{-1} &= 2\Delta \\ &\vdots \\ x_N + x_1^{-1} &= 2\Delta \end{aligned} \tag{30}$$

Using the alternative representation (13), we get $\Re(\lambda_j - \lambda_l) = 0$, for all j, l, which means the real parts of the λ_j coincide. For the imaginary parts we have

[5] They were first found by Baxter when considering the Q-T functional equations in ref. 4. In ref. 2 they were termed "exact complete N-strings." This terminology is somewhat misleading because a string is by definition a certain solution to the BA equations (10), which is not the case here.

$$\Im(\lambda_1-\lambda_2)=2+n_1\,\frac{2\pi}{\gamma}$$
$$\Im(\lambda_2-\lambda_3)=2+n_2\,\frac{2\pi}{\gamma}$$
$$\vdots \tag{31}$$
$$\Im(\lambda_N-\lambda_1)=2+n_N\,\frac{2\pi}{\gamma}$$

This entails

$$0=2N+\frac{2\pi}{\gamma}\sum_{i=j}^{N} n_j \qquad \text{or} \qquad \gamma=-\frac{\sum_{j=1}^{N} n_j}{N}\,\pi. \tag{32}$$

Because $0<\gamma<\pi$, we have $1\leqslant -\sum n_j = m_\gamma \leqslant N-1$. Using the non-uniqueness of the parameterization ($x_j=x(\lambda_j)=x(\lambda_j+2\pi in/\gamma)$ for n integer), we set the $n_j=0$ for $j=1,..., N-1$ and conclude $\lambda_1-\lambda_N=2i(N-1)$. Also note that the string we thus derived is exact—unlike the conventional one which involves exponential corrections.[5]

Usually one would write now for the N-string,

$$l_j=\lambda_0+(N+1-2j)\,i, \qquad j=1,..., N \tag{33}$$

yielding a string symmetric w.r.t the real axis. However, in our case the string can be shifted along the imaginary axis by an arbitrary value:

$$l_j=\lambda_0+ci+(N+1-2j)\,i, \qquad j=1,..., N \tag{34}$$

This incorporates the "odd parity string,"[8] but c is not restricted to the value π/γ.

This cbs-string is a transparent excitation, since from (34) and (13) it follows that:

$$S(\text{cbs}, \Lambda)=\prod_{j=1}^{N} S(\lambda_0+ic+(N+1-2j)\,i, \Lambda)=1 \tag{35}$$

for arbitrary Λ.

The total momentum P satisfies,

$$e^{iP}=\prod_j x(\lambda_0+ic+(N+1-2j)\,i), \tag{36}$$

so that

$$P = n\pi, \qquad \text{with} \quad n \equiv (m_\gamma + N) \bmod 2. \tag{37}$$

The total excitation energy for the cbs reads

$$E_{\text{cbs}} = 2\left(\sum_{j=1}^{N} \cos k_j^{\text{cbs}} - \Delta\right) = 0. \tag{38}$$

where the last equality follows from Eq. (30).

How many independent cyclic bound states are there? We note that the cbs-parameter $\lambda_0 + ic$ (or alternatively one of the k_j^{cbs}, say k_1^{cbs}) is *not* fixed by the periodic boundary conditions. The presence of other particles with arbitrary parameters k_l does not determine k_1^{cbs}, because of transparency, Eq. (35). It can therefore only be determined through the length L of the system. Let us write the wavefunction of the cbs above the reference state, without other particles:

$$f(n_1, \ldots, n_N) = A_1 x_1^{n_1} x_2^{n_2} \cdots x_N^{n_N} + A_2 x_2^{n_1} x_3^{n_2} \cdots x_1^{n_N} + \ldots A_N x_N^{n_1} x_1^{n_2} \cdots x_{N-1}^{n_N}. \tag{39}$$

Periodic boundary conditions lead to,

$$\begin{aligned} A_N &= A_1 x_N^L \\ A_1 &= A_2 x_1^L \\ &\vdots \\ A_{N-1} &= A_N x_{N-1}^L \end{aligned} \tag{40}$$

hence,

$$1 = \left(\prod_j^N x_j\right)^L \qquad \text{or} \qquad PL \equiv 0 \bmod 2\pi. \tag{41}$$

Hence for $P = \pi$, the cbs exist on chains with even length, and for $P = 0$, L is arbitrary. This remains the only restriction from periodicity. The cbs parameter $x_1 = e^{ik_1^{\text{cbs}}}$ is not fixed by any constraint and can be chosen as arbitrary complex number. This result is quite unusual, as one would expect all parameters of a Bethe state to be uniquely determined, apart from states corresponding to "roots at infinity." Indeed, in refs. 2 and 3, the attempt is made to find additional conditions determining the cbs parameter. We see now, that this not necessary. To the contrary: It is exactly the freedom to choose this parameter at will, which allows to find an analytical formula for the degeneracies in the spectrum caused by the presence of the cbs.

For each state $|\Psi\rangle$ given by a solution to (10), i.e., without cbs, there is in principle a continuous set of other states, having one or more additional cbs with parameters $x_1, x'_1, x''_1,...$. Only a finite number of them are linearly independent. The problem is then to determine the dimension of the "one-particle" Hilbert space, the number of linear independent cbs above the "parent" state $|\Psi\rangle$, i.e., in the sector with $S^z = S^z(\Psi) - N$. Because each cbs is transparent, it can be "added" to an arbitrary eigenstate $|\Psi(\{k_l^0\})\rangle$ of the hamiltonian without changing the BA equations for the parameters $\{k_l^0\}$ of $|\Psi\rangle$. In this way a new state $|\Psi'(\{k_l^0, k_j\})\rangle$ is created, which has the same energy as $|\Psi\rangle$ but different spin: $S^z(\Psi') = S^z(\Psi) - N$. Its rapidities are the cbs parameters $k_1,..., k_N$ and the rapidities $k_1^0,..., k^0_{L/2-S^z(\Psi)}$ of $|\Psi\rangle$. However, the amplitudes $A_P(\Psi')$ deviate in a complicated way from $A_P(\Psi)$, because the S-matrices between each member of the cbs and the excitations in $|\Psi(\{k_l^0\})\rangle$, $S(k_j, k_l^0)$, depend now not only on the set $\{k_j\}$ of the cbs but on $\{k_l^0\}$ as well. This is in contrast to the states generated by $U_q(sl_2)$, where these S-matrices are constant. The cbs apparently cannot be generated by an operator like (25). The coproduct structure of the quantum group allows only excitations having S-matrices which are independent of the spectral parameter. The same remains true for the affinization of $U_q(sl_2)$, $U_q(A_1^{(1)})$, but this question has to be further investigated.

The dimension of the "one-particle" cbs-multiplet built over a parent state $|\Psi\rangle$ (without any cbs) depends in general on the spin $S^z(\Psi)$ of the parent state $|\Psi\rangle$, as well as on the nature of parameters $k_1^0,..., k^0_{L/2-S^z(\Psi)}$ characterizing it, more specifically, whether or not exceptional momenta are present. We shall find that the parent states fall into three classes.

In the commensurable sectors the parent state can not contain the exceptional values $\pm k_q$ among the momenta $\{k_l^0\}$. However in an incommensurable sector with $S^z(\Psi) \equiv (N-m) \bmod N$, $m = 1,..., N-1$, the state $|\Psi\rangle$ may contain m momenta which are either all k_q or all $-k_q$.[6] Because the S-matrix for these excitations takes then the constant value (19), the number of independent cbs that can be added to $|\Psi\rangle$ is modified with respect to the case where the set $\{k_l^0\}$ contains no "exceptional" momenta $\pm k_q$.

Another way of having exceptional momenta in the parent state is in the form of m pairs of exceptional momenta with opposite sign, $\{k_q, -k_q\}$, added to the state $|\Psi_0\rangle$ to create a state $|\Psi\rangle$, degenerate with $|\Psi_0\rangle$. The BA equations for $|\Psi\rangle$ read,

[6] This possibility was pointed out to us by B. McCoy; these momenta manifest themselves as "roots at infinity" in the parameterization (12).

$$e^{-ik_l^0 L} = \prod_{l' \neq l}^{M'} S(k_l^0, k_{l'}^0)(q^{-2}q^2)^m$$

$$q^{-L} = (q^{-2})^{M'+m}$$

$$q^L = (q^2)^{M'+m}.$$

We have $S^z(\Psi_0) = L/2 - M'$ and $S^z(\Psi) = L/2 - M' - 2m$ from which follows,

$$S^z(\Psi_0) \equiv m \bmod N \qquad \text{and} \qquad S^z(\Psi) \equiv -m \bmod N. \tag{42}$$

This type of degeneracy can be reduced to the case where cbs excitations are present by using the Z_2-invariance of the spectrum with respect to flipping the z-component of all spins, $S^z \to -S^z$. Whereas the cbs-multiplets in commensurable sectors are mapped onto themselves by this transformation, there are two different multiplets in the incommensurable case, one corresponding to $S^z \equiv m \bmod N$, the other to $S^z \equiv -m \bmod N$. All states in the two sets are energetically degenerate. The states of the first set are generated from the reference state with all spins up and the members of the second are the spin-flipped states. From (42) we see that if $|\Psi_0\rangle$ belongs to the first set, $|\Psi\rangle$ belongs to the second and can be described as generated in the spin-flipped representation by adding one or more cbs to the state $|\Psi'_0\rangle$ with $S^z(\Psi'_0) = -S^z(\Psi_0)$. If we fix the representation (by using the spin-up reference state), the state $|\Psi\rangle$ can be regarded as parent state (because it is not a member of the multiplet generated from $|\Psi_0\rangle$) and adding one cbs to $|\Psi\rangle$ results again in a modification of the dimension formula as above.

We have therefore three different classes of degeneracies, depending on the presence of exceptional momenta in the parent state:

(I) The parent state contains no exceptional momenta. This is always the case for commensurable sectors.

(II) The parent state has $S^z(\Psi) \equiv m \bmod N$ $(m = 1, \ldots, N-1)$ and contains either $N-m$ equal momenta k_q or $N-m$ equal momenta $-k_q$.

(III) The parent state has $S^z(\Psi) \equiv m \bmod N$ $(m = 1, \ldots, N-1)$ and contains $N-m$ momenta k_q and $N-m$ momenta $-k_q$.

These three cases are the reason for the three types of degeneracies observed in the incommensurable sectors.[1] The case with independent numbers of k_q and $-k_q$ can not occur as is easily seen from the BA equations.

In the following we will concentrate on the case $N=3$. We have $\Delta=\pm 1/2$, corresponding to $\gamma=2\pi/3, \pi/3$. For $\Delta=1/2$, the cbs exist only on chains of even length L ($P=\pi$) and for $\Delta=-1/2$ on all chains ($P=0$).

We shall first determine the dimension dim $\mathscr{H}_1^0$ of the single-cbs space above the reference state $|0\rangle$ with all spins up, and subsequently the dimension of the single-cbs space dim $\mathscr{H}_1^\Psi$ built over a general state $|\Psi\rangle$. The amusing combinatorics is presented in Appendix A.2.

Our results are the following: The dimensionality of the cbs-space over $|0\rangle$ is,

$$\dim \mathscr{H}_1^0=\mu(L-2)+\iota(L-2), \tag{43}$$

where for an integer n we define the integers $\mu(n)\in\{0, 1, 2, 3,...\}$ and $\iota(n)\in\{0, 1, -1\}$ through the relation,

$$n=3\mu(n)+\iota(n). \tag{44}$$

The dimensionality of the degenerate space above a state $|\Psi\rangle$—different from the reference state—falls into the three cases discussed above,

Case I:

$$\dim \mathscr{H}_1^\Psi=\mu(2S^z(\Psi)-2)+\iota(2S^z(\Psi)-2). \tag{45}$$

Case II:

$$\dim \mathscr{H}_1^\Psi=\mu(2S^z(\Psi)-2)+\iota(2S^z(\Psi)-2)+1. \tag{46}$$

Case III:

$$\dim \mathscr{H}_1^\Psi=\mu(2S^z(\Psi)-2)+\iota(2S^z(\Psi)-2)+2. \tag{47}$$

Note that the dimension of dim $\mathscr{H}_1^\Psi$ in cases II and III do not depend on m, (which for $N=3$ may take the values 1 and 2). The derivation of (45)–(47) is also given in Appendix A.2.

Consider now states with two or more cbs. These correspond to multiplicities of type (5), (7) with $l>1$. Whereas it is possible in principle to determine the number of linear independent states containing l cbs over a state $|\Psi\rangle$ along the same lines as done for one cbs in Appendix A.2, there are many more entangled terms in the wavefunction and the calculation is very cumbersome. Because a mapping between the cbs and the states generated by $sl(2)$-loop is not known at present, we are unable to make contact with the program outlined in ref. 2, which attempts to use representation theory of this algebra to compute the dimensions of the multiplets in commensurable sectors.

Nevertheless, we wish to present the following argument, which renders formula (50) below at least plausible. Let us introduce the notion of the "effective size" of a particle and begin by illustrating its usefulness in computing the dimension of a degenerate space by applying it to the simple case of an XXX model. The dimension of the degenerate spaces of the XXX model is obtained by assuming that the "effective size" of each ordinary particle (spinless fermion/spin-down excitation) is two lattice sites while the "effective size" of a transparent excitation is not two but one lattice site, as follows from the fact that the number of allowed $k=0$ excitations which can be added to a state with M particles is then given by $L-2M$. We may add transparent excitations until the lattice is "completely filled." In other words, the "effective length" of the ring available for transparent excitations is reduced by an ordinary particle by two and by a transparent particle by one. Because $L-2M=2S^z_{\max}$, we find for the dimension of the $SU(2)$-multiplet, $2S^z_{\max}+1$ (including the parent state), which is correct, because the parent state is highest weight for $SU(2)$. That such a counting works is of course due to a non trivial property of the parent state, namely to be highest weight for the symmetry group $SU(2)$.

Lets assume now, that the same argument applies to the cbs symmetry. We have seen that the "effective length" of the ring entering formulas (45)–(47) for the one-cbs space is again $L-2M$. By analogy to the $SU(2)$ case we would conclude that the effective size of ordinary particles is 2 and the effective size for the cbs is 3—the minimal size for a three-particle excitation. Consider then a parent state $|\Psi\rangle$ with spin S^z and one additional cbs. To calculate the dimension for a second cbs, we have to take into account the reduction of the effective ring length $L_{\text{eff}}=L-2M=2S^z$ caused by the first cbs: $L'_{\text{eff}}=L_{\text{eff}}-3$. The dimension formula for the second cbs would read,

$$\mu(2S^z-3-2)+\imath(2S^z-3-2)=\dim\mathscr{H}_1^{\Psi}-1. \tag{48}$$

Because both cbs are indiscernible we have,

$$\dim\mathscr{H}_2^{\Psi}=\frac{\dim\mathscr{H}_1^{\Psi}(\dim\mathscr{H}_1^{\Psi}-1)}{2}. \tag{49}$$

Repeating this argument we conclude that if the one-cbs space has dimension $\dim \mathscr{H}_1^{\Psi}$, the number of available states for l cbs above the state $|\Psi\rangle$ reads:

$$\dim \mathscr{H}_l^{\Psi} = \binom{\dim \mathscr{H}_1^{\Psi}}{l}. \tag{50}$$

The dimension of a complete multiplet in the commensurable sector, $2^{l_{\max}}$ with $l_{\max} = \dim \mathscr{H}_1^{\Psi}$, follows then from (50) and formulae (45)–(47) for the single-particle space.

This argument does not constitute a proof of the binomial formula (50), as this would require in addition the demonstration that $|\Psi\rangle$ is highest weight for a (unknown) symmetry algebra different from $sl(2)$-loop, as our parent states are clearly *not* highest weight for this algebra.[2]

We wanted to draw attention to the curious fact, that such a simple counting indeed leads to the numerically observed multiplicities, not only for simple groups (as $SU(2)$), but even in the present case, where the underlying symmetry is much more complicated.

Let's return to the case with a single cbs and check Eq. (43). For $L \equiv 0 \bmod 3$, we have

$$\mu(L-2) = \frac{L}{3} - 1, \qquad \imath(L-2) = 1, \tag{51}$$

therefore, in the commensurable case,

$$\dim \mathscr{H}_1^0 = \frac{L}{3}, \tag{52}$$

in accord with (5). We give in Table I the number of states in the sector $S^z = L/2 - 3$, which are degenerate with the reference state, for L between 3 and 18 and $\Delta = -1/2$.

These (numerically confirmed) degeneracies coincide with the values predicted by (43) in the commensurable and incommensurable cases. Note

Table I. Number of States Degenerate with the Reference State in Sector $S^z = L/2 - 3$

L	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
$\deg(L/2-3)$	1	0	1	2	1	2	3	2	3	4	3	4	5	4	5	6

Table II. The Multiplicities deg(S^z) of the Reference State Energy in the Sectors with $S^z = S^z_{\max} - 3l$, and Lengths $L = 12$, 14, and 16. These Multiplicities Coincide with Formula (50) for More than One Cbs, i.e., with dim $\mathcal{H}^0_l$, in the Commensurable ($L = 12$) as Well as in the Incommensurable Cases ($L = 14$, 16)

L	energy	deg($L/2$)	deg($L/2-3$)	deg($L/2-6$)	deg($L/2-9$)	deg($L/2-12$)
12	3.0	1	4	6	4	1
14	3.5	1	4	6	4	1
16	4.0	1	4	6	4	1

the non-monotonic growth of the dimension of $\mathcal{H}^0_1$: e.g., for $L = 6$ there are two independent cbs, whereas for $L = 7$ there is only one independent state. As the reference state contains zero excitations, only case I above is relevant for commensurable and incommensurable chain lengths.

4. CONCLUSIONS

We have shown that the XXZ spin chain at roots of the unity admits a class of unusual excitations, the cyclic bound states. These excitations are transparent to other particles in the sense defined above and lead to a rich degeneracy pattern associated with some quantum symmetry. In particular we derived analytic expressions for the dimensionality of the degenerate spaces for $N = 3$ and $l = 1$.

The presence of transparent solutions indicates underlying symmetries. In particular the sl_2-loop symmetry contains generators $S^{-(N)}, T^{-(N)}$ which are associated with the special solution of (30) having all the $x_1 \cdots x_N$ equal: $x_1 = x_2 = \cdots x_N = q^{\pm 1}$. Applying $S^{-(N)}, T^{-(N)}$ to a state $|\Psi\rangle$ means adding N exceptional momenta $\pm k_q$. For these states both numerator and denominator of $S(k_j, k_{j+1})$ vanish, which means that $S(k_j, k_{j+1})$ has to be 1, not zero. This is the reason these states exist only in the commensurable sectors. However, they are linearly dependent on the general cbs: The states generated by sl_2-loop in the commensurable sectors are "singular" cyclic bound states. If they span the complete multiplet in the commensurable sectors, it must be possible to write the general cbs as superposition of the special states. As the explicit form of the states generated by $sl(2)$-loop is not known in general (see refs. 1–3) this question can not be answered at present.

The following tables contain some examples for the multiplets in the commensurable and incommensurable cases for chain lengths between 8 and 14. It is apparent, that formulas (45)–(47) describe only part of the degeneracies, namely that part, which is related to the cyclic bound states.

Table III. $L = 8$, $S^z_{\max} = 3$

energy	deg(3)	deg(0)
-1.0	1	2
-0.4142	2	4
1.0	2	4
2.4142	2	4
3.0	1	2

First, we note that some of the energies are two-fold degenerate already in the "parent sector," f.e. in Table III the energies -0.4142, 1.0, and 2.4142. This degeneracy is due to parity invariance, the two degenerate states have opposite momentum P. Accordingly, a factor of 2 multiplies the dimensions obtained from (45) in the sector $S^z = 0$.

This parity doubling occurs as well for several energies in Tables IV–X. Some energies show even a higher degeneracy in the parent sector: Energy 0.0 in Table IV, energy 0.5 in Table VI and energy 1.0 in Table VIII. This degeneracy of the parent states has to be taken into account, if one compares with formulae (45)–(47). Example: The energy 0.5 in Table VI is three-fold degenerate in the parent sector $S^z = 3$, formula (45) gives a degeneracy of 2 for each state in sector $S^z = 0$, which yields a total dimension of 6 for this energy in sector $S^z = 0$.

However, not *all* degeneracies can be explained by using the degeneracy of the parent states. F.e. energy 1.0 in Table VIII should be 10-fold degenerate in sector $S^z = 1$ and 5-fold degenerate in sector $S^z = -2$. Instead we find a 12-fold degeneracy for $S^z = 1$ and 9-fold for $S^z = -2$. These additional degenerate states are not due to the presence of cbs but have a different origin (which we do not know).

In any case the predicted degeneracies from the cbs give a lower bound to the number of energetically degenerate states.

Tables VII and VIII give examples for case II: There are two states with energy 3.0 in the sector $S^z_{\max} = 5$, corresponding to one-particle excitations with $\pm k_q$. They exist because $q^{12} = 1$. Formula (46) yields the degeneracy $2 + 1 = 3$ for each state in the sector $S^z = 5 - 3 = 2$ and (50) gives $\binom{3}{2} = 3$ in the sector $S^z = 5 - 6 = -1$, which coincides with the numerical results in Table VII. $S^z_{\max} = 4$ corresponds to two excitations in the parent state and we have again two states with energy 3.0. These are the states with (k_q, k_q), resp. $(-k_q, -k_q)$. The degeneracy in the sector with one cbs ($S^z = 1$) is again 3 and therefore the same in the sector with two cbs ($S^z = -2$). This is shown in Table VIII.

Table IV. $L = 8$, $S^z_{max} = 2$

energy	deg(2)	deg(−1)
−3.6389	1	0
−2.5615	2	0
−2.4142	2	0
−1.1579	1	0
−0.9318	2	2
−0.7320	2	2
0.0	3	4
0.4142	2	0
0.4823	2	2
1.0	1	0
1.5176	2	2
1.5615	2	0
2.0	1	2
2.7320	2	2
2.9318	2	2
3.7969	1	0

Table V. $L = 10$, $S^z_{max} = 4$

energy	deg(4)	deg(1)	deg(−2)
−0.5	1	2	1
−0.1180	2	4	2
0.8819	2	4	2
2.1180	2	4	2
3.1180	2	4	2
3.5	1	2	1

Table VI. $L = 10$, $S^z_{max} = 3$

energy	deg(3)	deg(0)	deg(−3)
−3.2756	1	2	1
−1.6318	1	2	1
0.0575	2	4	2
0.5	3	6	3
0.8847	1	2	1
1.5	1	2	1
4.3607	1	2	1

Table VII. $L = 12$, $S^z_{max} = 5$

energy	deg(5)	deg(2)	deg(−1)
0.0	1	4	3
0.2679	2	6	4
1.0	2	9	12
2.0	2	7	6
3.0	2	6	6
3.7320	2	6	4
4.0	1	2	1

Table VIII. $L = 12$, $S^z_{max} = 4$

energy	deg(4)	deg(1)	deg(−2)
0.1389	2	4	2
0.2383	1	2	1
1.0	5	12	9
2.0	1	6	7
3.0	2	6	6
4.0463	1	2	1
4.8983	1	2	1

Table IX. $L = 12$, $S^z_{max} = 3$

energy	deg(3)	deg(0)	deg(−3)
−5.3650	1	2	1
−4.6365	2	4	2
−3.6616	1	2	1
−1.8709	1	2	1
−1.0	1	8	1
−0.8904	1	2	1
0.6194	1	2	1

Table X. $L = 14$, $S^z_{\max} = 6$

energy	deg(6)	deg(3)	deg(0)	deg(-3)	deg(-6)
0.5	1	4	6	4	1
0.6980	2	8	12	8	2
1.2530	2	8	12	8	2
2.0549	2	8	12	8	2
2.9450	2	8	12	8	2
3.7469	2	8	12	8	2
4.3019	2	8	12	8	2
4.5	1	4	6	4	1

Table IV contains a state with a pair of exceptional momenta with opposite sign (case III), the state with energy 2.0 in sector $S^z_{\max} = 2$. The generic degeneracy in the sector $S^z = -1$ according to formula (45) is zero but the state with energy 2.0 possesses two states with $S^z = -1$, having the same energy, because Eq. (47) yields the value $0 + 2 = 2$ for the dimension of $\mathscr{H}^{\Psi}_{1}$.

APPENDIX A

A.1. Example: Adding Transparent Particles in the XXX-Chain

Take $l = 2$ and $M = 3$, then take some Q from $S(5)$, say:

$$Q = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 4 & 3 & 2 & 5 & 1 \end{pmatrix}$$

We want to construct a permutation P, which "coincides" with Q regarding the first three momenta k_1, k_2, k_3, i.e., $n(k_3) < n(k_2) < n(k_1)$. This is the permutation

$$P(Q) = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}$$

Now we apply formula (17). Compute first $P_{-1}(1)$: $Q^{-1}(1) = 5$. Now look for the preimages of 2 and 3 under Q: $Q^{-1}(2) = 3$ and $Q^{-1}(3) = 2$. Both are less than 5 (the preimage of 1) and therefore the number we are looking for is $2 + 1 = 3$. (Of course, the 1 itself with $Q^{-1}(1) = 5$ is counted as well.) It follows that $P^{-1}(1) = 3$.

Similar: because $Q^{-1}(2)=3$, there are two numbers k, less or equal to 3, for which $Q^{-1}(k)\leqslant Q^{-1}(2)$, namely 3, (with $Q^{-1}(3)=2<3$) and 2 itself. It follows $P^{-1}(2)=2$.

Again: As $Q^{-1}(3)=2$, there is only one index k which satisfies the condition $Q^{-1}(k)\leqslant Q^{-1}(3)=2$, namely 3 itself. Therefore $P^{-1}(3)=1$ and we get the wanted permutation $P(Q)$.

A.2. Derivation of Eqs. (43) and (45)–(47)

We confine ourselves here to the case $\Delta=1/2$, the case $\Delta=-1/2$ being completely analogous.

We begin by determining the parameters x_2, x_3 of the cbs in terms of $x_1=z$. From (30) we get

$$x_2=(1-z)^{-1}, \qquad x_3=1-z^{-1}. \tag{53}$$

To construct $\mathscr{H}_1^0$ we calculate the wavefunction of the cbs,

$$f(n_1,n_2,n_3;z)=A_1x_1^{n_1}x_2^{n_2}x_3^{n_3}+A_2x_2^{n_1}x_3^{n_2}x_1^{n_3}+A_3x_3^{n_1}x_1^{n_2}x_2^{n_3}. \tag{54}$$

We have (40),

$$A_1=1, \qquad A_2=x_1^{-L}, \qquad A_3=x_3^{L}. \tag{55}$$

It follows

$$\begin{aligned} f(n_1,n_2,n_3;z)=&(-1)^{n_3}\,z^{n_1-n_3}(1-z)^{n_3-n_2}\\ &+(-1)^{n_2}\,z^{n_3-n_2-L}(1-z)^{n_2-n_1}\\ &+(-1)^{L+n_1}\,z^{n_2-n_1-L}(1-z)^{L+n_1-n_3}. \end{aligned} \tag{56}$$

We see, that f is a certain meromorphic function in z, parameterized by the set of integers $\{n_1,n_2,n_3\}$ with $0\leqslant n_1<n_2<n_3\leqslant L-1$.

Now, as the parameter z is arbitrary, the question how many of the vectors $|\psi(z)\rangle=f(n_1,n_2,n_3;z)\,|n_1,n_2,n_3\rangle$ are linear independent, is equivalent to ask, how many of the functions $f(n_1,n_2,n_3;z)$, indexed by the set $\{n_1,n_2,n_3\}$, are linear independent over $\mathbb{C}$. (This follows from the equality of column rank and row rank of a matrix.)

We start out with a total of $\binom{L}{3}$ different functions $f(n_1,n_2,n_3;z)$. This is the maximal number of possible linear independent cbs states in the given sector of the Hilbert space. However, the set of really independent functions of type $f(n_1, n_2, n_3; z)$ is much smaller. First, we have the translation property, following from $P = \pi$. As one sees from (56), we have

$$f(n_1, n_2, n_3; z) = -f(n_1+1, n_2+1, n_3+1; z). \tag{57}$$

Therefore, we can fix $n_1 = 0$. Furthermore, we put

$$\begin{aligned} n_2 - 1 &= i \\ n_3 - n_2 - 1 &= j \\ L - n_3 - 1 &= k \end{aligned}$$

we have $i + j + k = L - 3$ and $0 \leqslant i, j, k \leqslant L - 3$. Then

$$f(i, j, k; z) = \frac{z(z-1)}{z^L} \phi(i, j, k; z) \tag{58}$$

with

$$\phi(i, j, k; z) = (z-1)^i z^j - (-1)^i (z-1)^j z^k + (-1)^j (z-1)^k (-z)^i. \tag{59}$$

Now one confirms that

$$\phi(i+1, j, k; z) = \phi(i, j+1, k; z) - \phi(i, j, k+1; z). \tag{60}$$

We can, without loss of generality, put $i = 0$. Lets look at the polynomials

$$\varphi_j(z) = \phi(0, j, L-3-j; z) = z^j - (z-1)^j z^{L-3-j} - (1-z)^{L-3-j}, \tag{61}$$

$j = 0, \ldots, L-3$, the sign of the last summand is negative because L is even. The maximal number of independent states is reduced in this way to $L-2$. However, the set $\{\varphi_j(z)\}_{j=0,\ldots,L-3}$ is not linear independent. There are further relations among the polynomials. Lets form the expression

$$\Phi(x, z) = \sum_{j=0}^{L-3} x^j \varphi_j(z) \binom{L-3}{j}. \tag{62}$$

This is a way to shift the dependence on j over to the (complex) parameter x. We find:

$$\Phi(x, z) = (xz+1)^{L-3} - ((x+1) z - x)^{L-3} - (x+1-z)^{L-3}. \tag{63}$$

What relations are possible among the functions $\Phi(x, z)$? We make the ansatz,

$$\Phi(x, z) = \sum_r \alpha_r \Phi(\tilde{x}_r, z). \tag{64}$$

By examination of (63) and (64) one sees that all possible relations of this type reduce to the following:

$$\Phi(x, z) = \alpha^{L-3} \Phi(\tilde{x}, z). \tag{65}$$

To solve (65) identical in z, we must have

$$\begin{aligned} xz+1 &= -\alpha((\tilde{x}+1)\, z - \tilde{x}) \\ (x+1)\, z - x &= \alpha(\tilde{x}+1-z) \\ x+1-z &= -\alpha(\tilde{x}z+1), \end{aligned} \tag{66}$$

and

$$\tilde{x} = -\frac{1}{x+1}, \qquad \alpha = -(1+x). \tag{67}$$

Then

$$\Phi(x, z) = -(1+x)^{L-3}\, \Phi(-(1+x)^{-1}, z). \tag{68}$$

Going now back to (62), we can write (68) as

$$\sum_{j=0}^{L-3} c_j(x)\, \tilde{\phi}_j(z) = 0, \tag{69}$$

with

$$c_j(x) = x^j - \frac{(-1)^{j+1}}{(1+x)^j}\,(1+x)^{L-3}, \qquad \tilde{\varphi}_j(z) = \binom{L-3}{j}\, \varphi_j(z), \tag{70}$$

for arbitrary x. Because relation (69) is valid for all x, we conclude that

$$\dim\langle\{\varphi_j(z)\}_{j=0,\dots,L-3}\rangle + \dim\langle\{c_j(x)\}_{j=0,\dots,L-3}\rangle \leqslant L-2, \tag{71}$$

$\langle\cdots\rangle$ denotes the linear span. But because *all* linear relations among the $\Phi(x, z)$ can be reduced to (65), we have actually

$$\dim\langle\{\varphi_j(z)\}\rangle + \dim\langle\{c_j(x)\}\rangle = L-2. \tag{72}$$

By choosing the basis $x^0, x^1, \ldots, x^{L-3}$ to span $\langle\{c_j(x)\}\rangle$, we find that its dimension is equal to the rank of the $(L-2)\times(L-2)$-matrix

$$\mathbb{1} - A_{L-3}, \tag{73}$$

with

$$A_n(i,k) = (-1)^{i+n}\binom{n-i}{k}, \tag{74}$$

for $i, k = 0, \ldots, n$. The $(n+1)\times(n+1)$-matrices A_n, we call Pascal matrices, for obvious reasons. (We have defined $\binom{n}{m} = 0$ if $m > n$) The matrix A_3, f.e. reads

$$A_3 = \begin{pmatrix} -1 & -3 & -3 & -1 \\ 1 & 2 & 1 & 0 \\ -1 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{75}$$

The Pascal matrices have interesting properties, intimately connected with our problem. Lets define the inversion Matrix S_n through

$$S_n(i,k) = \delta_{i,\,n-k} \tag{76}$$

for $i, k = 0, \ldots, n$. Then we can show by induction

$$S_n A_n S_n = A_n^{-1} = A_n^2, \tag{77}$$

from which we have $A_n^3 = \mathbb{1}$. From this follows, that A_n is diagonalizable. Moreover we have for the trace of A_n:

$$\operatorname{tr} A_n = \imath(n+1) \tag{78}$$

(compare (44)). These identities for the Pascal matrices are equivalent to the combinatorial identities

$$\sum_{k=0}^{n} (-1)^k \binom{n-i}{k}\binom{n-k}{l} = \binom{i}{n-l}, \tag{79}$$

$$\sum_{k=0}^{n} (-1)^{i+k+n} \binom{n-i}{k}\binom{k}{n-l} = \delta_{il}, \tag{80}$$

and

$$(-1)^n \sum_{k=0}^{n} (-1)^k \binom{n-k}{k} = \imath(n+1). \tag{81}$$

Now we can compute the characteristic polynomial of A_n for all $n = 0, 1,\ldots$. (This is relevant for $\Delta = 1/2$ only for odd n, but for $\Delta = -1/2$, all n are needed.) We write

$$(-1)^{n+1} \det(A_n - \lambda \mathbb{1}) = \det(\lambda \mathbb{1} - A_n)$$

and use

$$\ln \det(\lambda \mathbb{1} - A_n) = \mathrm{tr}[\ln(\lambda \mathbb{1} - A_n)].$$

Expanding the log, we have,

$$\ln(\lambda \mathbb{1} - A_n) = \ln(\lambda \mathbb{1}) - \sum_{i=1}^{\infty} \frac{\lambda^{-i}}{i} A_n^i, \tag{82}$$

and with relations (77)

$$\sum_{i=1}^{\infty} \cdots = \frac{A_n}{\lambda} + \frac{1}{2} \frac{S_n A_n S_n}{\lambda^2} + \frac{1}{3} \frac{\mathbb{1}}{\lambda^3} + \frac{1}{4} \frac{A_n}{\lambda^4} + \frac{1}{5} \frac{S_n A_n S_n}{\lambda^5} + \frac{1}{6} \frac{\mathbb{1}}{\lambda^6} + \cdots \tag{83}$$

With (78), $\mathrm{tr}(S_n A_n S_n) = \mathrm{tr}(A_n)$ and $\mathrm{tr}\, \mathbb{1} = n+1$, it follows

$$\mathrm{tr}\left(\sum_{i=1}^{\infty} \frac{\lambda^{-i}}{i} A_n^i \right) = (n+1) \sum_{i \in I_3} \frac{\lambda^{-i}}{i} + \imath(n+1) \sum_{i \notin I_3} \frac{\lambda^{-i}}{i}. \tag{84}$$

The index set I_3 contains all multiples of 3: $I_3 = 3, 6, 9,\ldots$. Using now $n+1 = 3\mu(n+1) + \imath(n+1)$, we rewrite the first sum on the r.h.s of (84) as,

$$(\mu + \imath/3) \sum_{j=1}^{\infty} \frac{(\lambda^{-3})^j}{j} = -(\mu + \imath/3) \ln(1 - \lambda^{-3}) \tag{85}$$

and the second sum,

$$\imath \left[\sum_{j=1}^{\infty} \frac{\lambda^{-j}}{j} - (1/3) \sum_{j=1}^{\infty} \frac{(\lambda^{-3})^j}{j} \right]. \tag{86}$$

Adding both terms and inserting into (82) we find,

$$\mathrm{tr}(\ln(\lambda\mathbb{1}-A_n)) = \mu(n+1)[3\ln\lambda+\ln(1-\lambda^{-3})]+\imath(n+1)[\ln\lambda+\ln(1-\lambda^{-1})] \tag{87}$$

and finally,

$$\det(A_n-\lambda\mathbb{1}) = (-1)^{n+1}\,[(\lambda^3-1)^{\mu(n+1)}\,(\lambda-1)^{\imath(n+1)}]. \tag{88}$$

From (88) we have the dimension of the eigenspace to the eigenvalue 1: $\mu(n+1)+\imath(n+1)$, (remember that A_n is diagonalizable). And this entails, in view of (72) and (73), that

$$\dim\langle\{\varphi_j(z)\}\rangle = \dim\mathscr{H}_1^0 = \mu(L-2)+\imath(L-2). \tag{89}$$

Now we consider the case $S^z(\Psi) < L/2$. First, assume that only one excitation is present:

$$|\Psi\rangle = \sum_{n=0}^{L-1} x_0^n\,|n\rangle, \tag{90}$$

with $x_0^L = 1$ and $x_0 \neq q^{\pm 1}$ (case I). The wavefunction with one cbs on top of the single particle state $|\Psi\rangle$ reads

$$|\Psi'\rangle = \sum_{0\leqslant n_0<n_1<n_3<L} f(n_0,n_1,n_2,n_3)\,|n_0,n_1,n_2,n_3\rangle \tag{91}$$

with

$$\begin{aligned} f(n_0,n_1,n_2,n_3) = {} & x_0^{n_0}x_1^{n_1}x_2^{n_2}x_3^{n_3} + S_{01}x_1^{n_0}x_0^{n_1}x_2^{n_2}x_3^{n_3} + S_{30}x_1^{n_0}x_2^{n_1}x_0^{n_2}x_3^{n_3} \\ & + x_1^{n_0}x_2^{n_1}x_3^{n_2}x_0^{n_3} + S_{01}x_0^{n_0}x_2^{n_1}x_3^{n_2}x_1^{n_3-L} + S_{30}x_2^{n_0}x_0^{n_1}x_3^{n_2}x_1^{n_3-L} \\ & + x_2^{n_0}x_3^{n_1}x_0^{n_2}x_1^{n_3-L} + S_{01}x_2^{n_0}x_3^{n_1}x_1^{n_2-L}x_0^{n_3} + S_{30}x_0^{n_0}x_3^{n_1+L}x_1^{n_2}x_2^{n_3} \\ & + x_3^{n_0+L}x_0^{n_1}x_1^{n_2}x_2^{n_3} + S_{01}x_3^{n_0+L}x_1^{n_1}x_0^{n_2}x_2^{n_3} + S_{30}x_3^{n_0+L}x_1^{n_1}x_2^{n_2}x_0^{n_3} \end{aligned} \tag{92}$$

with the S-matrices

$$S_{01} = -\frac{(x_0-1)\,z+1}{(z-1)\,x_0+1}, \qquad S_{30} = \frac{x_0-z}{(z-1)\,x_0+1}. \tag{93}$$

Lets define

$$
\begin{aligned}
a &= n_1 - n_0 \\
b &= n_2 - n_1 \\
c &= n_3 - n_2 \\
d &= L + n_0 - n_3,
\end{aligned}
\tag{94}
$$

with $1 \leqslant a, b, c, d \leqslant L-3$, $a+b+c+d=L$. The polynomial $f'(n_0, n_1, n_2, n_3; x_0, z) = z^L[(z-1)\, x_0 + 1]\, f(n_0, n_1, n_2, n_3)$ can be written as

$$
\begin{aligned}
f'(n_0, n_1, n_2, n_3; x_0, z) = (-x_0)^{n_0}\, &[(-1)^{b+a}\, \phi(c, L-b-c, b+1; z) \\
&+ x_0(-1)^d\, \phi(L-b-c, b, c+1; z)] \\
&+ (-x_0)^{n_1}\, [(-1)^{c+b}\, \phi(d, L-d-c, c+1; z) \\
&+ x_0(-1)^a\, \phi(L-d-c, c, d+1; z)] \\
&+ (-x_0)^{n_2}\, [(-1)^{d+c}\, \phi(a, L-a-d, d+1; z) \\
&+ x_0(-1)^b\, \phi(L-a-d, d, a+1; z)] \\
&+ (-x_0)^{n_3}\, [(-1)^{a+d}\, \phi(b, L-a-b, a+1; z) \\
&+ x_0(-1)^c\, \phi(L-a-b, a, b+1; z)].
\end{aligned}
\tag{95}
$$

One sees, that f' lies in the span of the functions $\phi(i, j, k; z)$, with $i+j+k = L+1$ and $i = 1,..., L-3$; $j, k = 2,..., L-2$, respectively $j = 1,..., L-3$ and $i, k = 2,..., L-2$. The second case can be reduced to the first with the aid of the relation

$$
\phi(i, j, k; z) = (-1)^{i+1}\, \phi(j, k, i; z). \tag{96}
$$

Moreover, using (60) and (96), one can show that

$$
\dim\langle \{\phi(i, j, k; z)\} \mid i \geqslant 1;\, j, k \geqslant 2 \rangle = \dim\langle \{\phi(i, j, k; z)\} \mid i, j, k \geqslant 1 \rangle. \tag{97}
$$

Lets write $\langle \{\phi(i, j, k; z)\} \mid i, j, k \geqslant 1 \rangle = \mathscr{H}'$. Repeating the arguments above, we have

$$
\dim \mathscr{H}' = \mu(L-1) + \iota(L-1). \tag{98}
$$

Now for the dimension of $\mathscr{H}_1^{\Psi} = \langle f'(n_0, n_1, n_2, n_3; x_0, z) \rangle$ we have

$$
\dim \mathscr{H}_1^{\Psi} = \dim \mathscr{H}' - 1, \tag{99}
$$

because the functions of type (95) do not span all of $\mathscr{H}'$: they satisfy an additional relation coming from the fact, that $x_0^L = 1$, i.e., that $|\Psi\rangle$ is an eigenstate of the hamiltonian. To prove this, assume the contrary, $\mathscr{H}' \subset \mathscr{H}_1^\Psi$. Then one could write

$$f'(n_0, n_1, n_2, n_3; \tilde{x}, z_0) = \sum_k \alpha_k f'(n_0, n_1, n_2, n_3; x_0, z_k) \tag{100}$$

with *arbitrary* $\tilde{x}$ and z_0 for some z_k and all $\{n_0, n_1, n_2, n_3\}$. But this is impossible, because all the $f'(n_0, n_1, n_2, n_3; x_0, z_k)$ satisfy the periodicity condition

$$f'(0, n_1, n_2, n_3; x_0, z_k) = f'(n_1, n_2, n_3, L; x_0, z_k) \tag{101}$$

whereas this is not true for $f'(n_0, n_1, n_2, n_3; \tilde{x}, z_0)$ if $\tilde{x}^L \neq 1$. This additional relation is a reflection of the fact, that $|\Psi'\rangle$ satisfies exactly one BA equation (10). Besides this one, there is no other relation among the functions f' because x_0 can now be considered as a free parameter in (95). In an analogous way, r excitations in $|\Psi\rangle$, with parameters $x_0, x_1, \ldots, x_{r-1}$, lead for $\mathscr{H}'$ to the dimension formula,

$$\dim \mathscr{H}' = \mu(L-2+r) + \imath(L-2+r) \tag{102}$$

and

$$\dim \mathscr{H}_1^\Psi = \dim \mathscr{H}' - r, \tag{103}$$

because now $|\Psi\rangle$ and $|\Psi'\rangle$ satisfy r BA equations. Eq. (103) can be written in another way, by observing that

$$\mu(n+3m) - \mu(n) = m, \qquad \imath(n+3m) = \imath(n),$$

for all $n, m \geqslant 1$. It follows

$$\dim \mathscr{H}_1^\Psi = \mu(L-2-2r) + \imath(L-2-2r) = \mu(2S^z(\Psi)-2) + \imath(2S^z(\Psi)-2). \tag{104}$$

This completes the proof of (45) corresponding to case I.

For case II we set $x_0 = q$. To have $x_0^L = 1$, L must be divisible by 3. Now, instead of (93), we have

$$S_{01} = q^{-2}, \qquad S_{30} = q^2. \tag{105}$$

These S-matrices do not depend on z, which allows to write for the component of $f(n_0, n_1, n_2, n_3)$ multiplying $x_0^{n_0}$:

$$\tilde{f}(a, b, c, d; q, z) = z^{-L}[(-1)^{a+b+c} z^{d+a}(1-z)^c + q^{-2}(-1)^{a+b} z^c(1-z)^b + q^2(-1)^{L+a} z^b(1-z)^{d+a}], \tag{106}$$

where we have used convention (94). Cyclic permuted expressions are obtained for the components of f multiplying $x_0^{n_i}$, $i=1, 2, 3$. To compute $\dim \mathscr{H}'$, consideration of $\tilde{f}$ in (106) is sufficient. We have,

$$\tilde{f} = (-1)^a z^{-L} \phi_q(i, j, k; z), \tag{107}$$

with

$$\phi_q(i, j, k; z) = q^{-2}(z-1)^i z^j + (-1)^i (z-1)^j z^k + q^2(-1)^j (z-1)^k (-z)^i, \tag{108}$$

with $i+j+k=L$; $i, j=1,..., L-3$; $k=2,..., L-2$. The polynomials $\phi_q(i, j, k; z)$ fulfill relation (60) and (96) reads now

$$\phi_q(j, k, i; z) = (-1)^i q^{-2} \phi_q(i, j, k; z), \tag{109}$$

because $q^6=1$. From these relations we have

$$\begin{aligned}&\dim\langle\{\phi_q(i, j, k; z) \mid i, j \geqslant 1; k \geqslant 2\}\rangle \\ &\quad = \dim\langle\{\phi_q(i, j, k; z) \mid i, j, k \geqslant 1\}\rangle = \dim \mathscr{H}'.\end{aligned} \tag{110}$$

$\mathscr{H}'$ is spanned by functions

$$\varphi_{qj}(z) = q^{-2} z^j - (z-1)^j z^{L-3-j} - q^2(1-z)^{L-3-j}, \tag{111}$$

with $j=0,..., L-3$. The analogue to (63) reads,

$$\Phi_q(x, z) = q^{-2}(xz+1)^{L-3} - ((x+1) z - x)^{L-3} - q^2(x+1-z)^{L-3}. \tag{112}$$

The functional relation $\Phi_q(x, z) = \alpha^{L-3} \Phi_q(\tilde{x}, z)$ is solved by

$$\begin{aligned} q^{-2}(xz+1) &= -p_1\alpha((\tilde{x}+1) z - \tilde{x}) \\ (x+1) z - x &= p_2\alpha q^2(\tilde{x}+1-z) \\ q^2(x+1-z) &= -p_3\alpha q^{-2}(\tilde{x}z+1), \end{aligned} \tag{113}$$

with numbers $p_{1,2,3}$, satisfying $p_i^{L-3}=1$. As 3 divides $L-3$ we can choose $p_1=p_2=p_3=q^{-2}$, which yields the solution (67) for α and $\tilde{x}$. We conclude,

$$\dim \mathscr{H}' = \mu(L-2)+\imath(L-2), \tag{114}$$

and for a state $|\Psi\rangle$ containing M' ordinary and one exceptional momentum,

$$\dim \mathscr{H}' = \mu(L-2+M')+\imath(L-2+M'). \tag{115}$$

Because we have still $M'+1$ independent BA equations, it follows

$$\dim \mathscr{H}_1^{\Psi} = \dim \mathscr{H}' - M' - 1 = \frac{2S^z+1}{3} - 1, \tag{116}$$

with $S^z = L/2 - M' - 1 \equiv -1 \bmod 3$. This can be written as

$$\dim \mathscr{H}_1^{\Psi} = \mu(2S^z-2)+\imath(2S^z-2)+1, \tag{117}$$

which is formula (46). Now we assume $m=2$, the state $|\Psi\rangle$ contains two exceptional momenta of equal sign and M' ordinary momenta. By an argument, which parallels the discussion above, we find for $\dim \mathscr{H}'$:

$$\dim \mathscr{H}' = \mu(L-2+M')+\imath(L-2+M'). \tag{118}$$

But now the number of independent BA equation is not $M'+2$ but $M'+1$, as the two exceptional momenta are indiscernible. Therefore,

$$\dim \mathscr{H}_1^{\Psi} = \dim \mathscr{H}' - M' - 1 = \frac{2S^z+2}{3} - 1. \tag{119}$$

Now, $S^z \equiv 1 \bmod 3$, and we find again formula (46), which is therefore independent of m.

Case III can be treated without recourse to the wavefunction, by using the Z_2 symmetry of the spectrum. Assume the state $|\Psi\rangle$ contains one momentum k_q and one momentum $-k_q$. It is therefore degenerate with a state $|\Psi_0\rangle$ (we use the notation of Section 3) having $S^z(\Psi_0) = S^z(\Psi)+2$. Whereas $S^z(\Psi) \equiv -1 \bmod 3$, $S^z(\Psi_0) \equiv 1 \bmod 3$. We look for the state $|\Psi'\rangle$ in the multiplet of $|\Psi_0\rangle$ having $S^z(\Psi') = -S^z(\Psi)$ and determine the number k of cbs, which have to be added to $|\Psi_0\rangle$ to reach $|\Psi'\rangle$: $S^z(\Psi_0) - 3k = S^z(\Psi')$. We find

$$k = \frac{S^z(\Psi_0)+S^z(\Psi)}{3} = \frac{2S^z(\Psi)+2}{3}. \tag{120}$$

Now, by Z_2 symmetry,

$$\dim \mathcal{H}_1^{\Psi} = \dim \mathcal{H}_{k-1}^{\Psi_0} = \binom{\dim \mathcal{H}_1^{\Psi_0}}{k-1}, \tag{121}$$

where we have assumed (50). Because $|\Psi_0\rangle$ contains no exceptional momenta, we have

$$\dim \mathcal{H}_1^{\Psi_0} = \mu(2S^z(\Psi)+2) + \imath(2S^z(\Psi)+2) = \frac{2S^z(\Psi)+2}{3} = k. \tag{122}$$

$|\Psi'\rangle$ is therefore uniquely determined and

$$\dim \mathcal{H}_1^{\Psi} = \binom{k}{k-1} = k = \dim \mathcal{H}_1^{\Psi_0}. \tag{123}$$

Because

$$\mu(2S^z(\Psi)-2) + \imath(2S^z(\Psi)-2) = \frac{2S^z(\Psi)+2}{3} - 2, \tag{124}$$

we find formula (47). For the case with four additional exceptional momenta, we have $S^z(\Psi) \equiv 1 \bmod 3$ and $S^z(\Psi_0) \equiv -1 \bmod 3$, $S^z(\Psi_0) = S^z(\Psi) + 4$ and $k = (2S^z(\Psi)+4)/3$. We have $\dim \mathcal{H}_1^{\Psi_0} = \dim \mathcal{H}_1^{\Psi} = k$ as above and find because $\mu(2S^z(\Psi)-2) + \imath(2S^z(\Psi)-2)$ is now $(2S^z(\Psi)-2)/3$ again formula (47), independent of m. This concludes the derivation of (43) and (45)–(47).

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