Exact S-matrices for $d_{n+1}^{(2)}$ affine Toda solitons and their bound states

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ABSTRACT

We conjecture an exact S-matrix for the scattering of solitons in $d_{n+1}^{(2)}$ affine Toda field theory in terms of the R-matrix of the quantum group $U_q(c_n^{(1)})$. From this we construct the scattering amplitudes for all scalar bound states (breathers) of the theory. This S-matrix conjecture is justified by detailed examination of its pole structure. We show that a breather-particle identification holds by comparing the S-matrix elements for the lowest breathers with the S-matrix for the quantum particles in real affine Toda field theory, and discuss the implications for various forms of duality.

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1 Introduction

The Lagrangian density of affine Toda field theory (ATFT) with imaginary coupling-constant (‘imaginary ATFT’) can be written in the form

\[ \mathcal{L} = \frac{1}{2} (\partial_\mu \phi)(\partial^\mu \phi) + \frac{m^2}{\beta^2} \sum_{j=0}^{n} n_j (e^{i\beta \alpha_j \cdot \phi} - 1). \] (1)

The field \( \phi(x, t) \) is an \( n \)-dimensional vector, \( n \) being the rank of the finite Lie algebra \( g \). The \( \alpha_j \) (\( j = 1, \ldots, n \)) are the simple roots of \( g \); \( \alpha_0 \) is chosen such that the inner products among the elements of the set \( \{ \alpha_0, \alpha_j \} \) are described by one of the extended Dynkin diagrams of an affine algebra \( \hat{g} \). It is expressible in terms of the other roots by

\[ \alpha_0 = -\sum_{j=1}^{n} n_j \alpha_j \]

where the \( n_j \) are positive integers, and \( n_0 = 1 \). \( \beta \) is a coupling constant (which in the notation here is a positive real number) and \( m \) a mass scale. We take the roots to be normalised so that \( \text{longest root}^2 = 2k \), where \( k \) is the twist of the affine algebra.

Four years ago Hollowood discovered classical soliton solutions [1] to \( a_n^{(1)} \) imaginary ATFTs. Solitons were subsequently found for ATFTs based on other algebras [2], and a general construction based on vertex operators followed [3]. For algebras other than \( a_n^{(1)} \) (when the ATFT is the sine-Gordon model), the Hamiltonian is complex; yet the solitons have real energy and momenta, and real higher conserved charges [4]. The solitons fall into species labelled (for untwisted affine algebras) by spots on the Dynkin diagram of \( g \), and have topological charges which lie in, but by no means fill, the fundamental representations of \( g \) [5]. (It has to be hypothesised that in the quantum theory states exist which fill the quantized affine algebra representations.) Further, like the sine-Gordon model, these theories have continuous spectra of bound states with zero topological charge (‘breathers’) of each species; but, unlike the sine-Gordon model, there are also similar states with non-zero charge (‘excited solitons’ or ‘breathing solitons’) [6].

Using the semiclassical methods of [7] the order \( \beta^2 \) quantum mass corrections have been calculated [8, 9, 10] and the semiclassical limit of the \( S \)-matrix computed [11]. However, the \( \hat{g} \) ATFT has as a dynamical symmetry an underlying \( U_q(\hat{g}^\vee) \) charge algebra [12, 13] (where the superscript denotes the dual of \( \hat{g} \), i.e. the algebra obtained by replacing all the roots with co-roots, \( \alpha \mapsto \frac{2}{\alpha} \alpha \)), and conservation of these charges allows us to solve for the
exact soliton $S$-matrix, which satisfies the Yang-Baxter equation (YBE). This was done for the $a_n$ case in [14].

In the quantum theory the mass spectrum of the excitations becomes discrete, and in the sine-Gordon theory it is natural to identify the lowest breather state with the quantum particle (the quantized vacuum excitation). This seems to apply more generally: comparing with the mass and $S$-matrix calculations for the particles carried out in [13, 14] for the real coupling case ($\beta$ purely imaginary in [1]), which we shall call ‘real ATFT’ [3], we find that, when $\hat{g}$ is self-dual, the lowest breather masses implied by the semiclassical soliton mass corrections and the exact $S$-matrix poles are precisely those of the particles [9, 10]. Further, in the only case investigated in detail ($a_2^{(1)}$ in [18]) the $S$-matrix also matches.

The theories based on self-dual affine algebras (the simply-laced algebras plus $a_{2n}^{(2)}$) are the least interesting, in that the classical mass ratios for solitons, breathers and particles are unaltered by quantum mass corrections. In contrast, for nonsimply-laced $\hat{g}$ the relations among the masses and $S$-matrices of these objects are little understood. The nonsimply-laced $\hat{g}$ fall into two categories, both of which may be obtained from simply-laced theories as subspaces invariant under automorphisms (‘foldings’) of the extended Dynkin diagram. For the twisted algebras (i.e. where the automorphism involves the extended root) both particles and solitons are a subset of those of the parent theory. Their masses, however, now renormalise differently, although the corrections are in the same ratio for solitons and particles of the same species. Any attempt to construct exact $S$-matrices must take account of this fact via the introduction of flexible pole structure, the possibility of which has only recently been recognised [19]. The least tractable case is that of the untwisted nonsimply-laced algebras (i.e. where the automorphism does not involve the extended root), where even the classical masses of the solitons and particles are not proportional: in fact, the masses of the solitons of the ATFT based on (the affine extension of) $g$ are proportional to those of the particles of the $g^\vee$ ATFT [3], a fact suggestive of some kind of ‘Lie duality’ (in contrast to the ‘affine duality’ found [15, 21] between the particles of the $\hat{g}$ real ATFT in the weak-coupling regime and those of the $\hat{g}^\vee$ theory in the strong regime). However, this can only be made to work in a rather subtle way in the quantum theory: if we assume that the ratios of the quantum masses to the classical masses of solitons and particles of the same species are independent of the species (even for untwisted nonsimply-laced $\hat{g}$, where the ratios of the classical masses depend on the species)\footnote{For a recent review of real ATFT see [17].}, then this duality persists only\footnote{See [8, 10] and the discussions therein: this assumption will hold only if the naïve semiclassical approach fails.}.
between imaginary-coupled solitons and real-coupled particles.

It is only feasible to construct exact S-matrices where the spectral decomposition of the $U_q(\hat{g}^{\vee})$-invariant solutions of the YBE ('$R$-matrices') is known for all species. This is only the case for those algebras for which the fundamental representations of $U_q(\hat{g}^{\vee})$ are irreducible as representations of the Lie subalgebra; and this is only true where the Lie algebra is $a_n$ or $c_n$. The $a_n$ case has been investigated by Hollowood [14], who examined the soliton S-matrices but did not fuse them to obtain breather or excited soliton S-matrices, which are in some ways rather subtle because of the non-self-conjugacy of the particles and solitons. The $a_2^{(1)}$ case has been investigated in detail [18]. In this paper we investigate the $d_n^{(2)}$ ATFTs, which therefore have $U_q(c_n^{(1)})$ symmetry and $U_q(c_n)$-invariant S-matrices. We construct soliton-soliton S-matrices, and from them construct the breather-soliton, breather-breather and breather-excited soliton S-matrices, although the excited soliton-excited soliton S-matrices remain beyond our scope.

In section two we gather together some necessary facts about $U_q(c_n)$-invariant R-matrices, and in section three we fuse the soliton S-matrices to obtain S-matrices for the breather bound states, finding that those for the lowest breather states are precisely those for the particles [21], supporting the identification of these objects. In section four we investigate the soliton S-matrices’ pole structure and present what we believe to be the minimal set of three-point couplings necessary for the bootstrap to close.

This paper, dealing with a twisted theory, should be seen as an intermediate step between the simply-laced theories and the untwisted nonsimply-laced theories, which will be the subject of future work. In section five we expand on our discussion above and present a general scheme for the investigation of these theories and of affine and Lie duality. Four appendices deal, respectively, with generalisation to other algebras, details of crossing symmetry for the basic $R$-matrix, details necessary for the calculation of the scalar factor in the $S$-matrix, and the pole structure of the (rational) $c_n$-invariant S-matrices.
2 $U_q(c_n)$-invariant $R$-matrices

The $U_q(c_n)$-invariant $R$-matrices can be described using the tensor product graph [22, 23] and are given by [24, 25, 26]

$$\tilde{R}^{(TPG)}_{a,b}(x) = \sum_{p=0}^{\min(b,n-a)} \sum_{r=0}^{b-p} \prod_{i=1}^{p} \langle a - b + 2i \rangle \prod_{j=1}^{r} (2n + 2 - a - b + 2j) \hat{P}_{\lambda_{a+p-r}+\lambda_{b-p-r}}$$

in which $a, b = 1, \ldots, n$; $a \geq b$ and $\langle k \rangle = \frac{1-xq^k}{x-q^k}$. $\hat{P}_{\lambda}$ denotes the projector onto the ($q$-deformation of the) module of the irreducible $c_n$-representation with highest weight $\lambda$ (which we shall denote $V_i$ when $\lambda = \lambda_i$, the $i$th fundamental weight; $\lambda_0 \equiv 0$). $\tilde{R}^{(TPG)}_{a,b}(x)$ acts as an intertwiner on these modules

$$\tilde{R}^{(TPG)}_{a,b}(x) : V_a \otimes V_b \rightarrow V_b \otimes V_a$$

The tensor product graph (TPG) itself, in which the coefficients of two linked representations in the graph are in the ratio $\langle \Delta \rangle$ where $\Delta$ is the difference in the two values of the quadratic Casimir operator, is

$$\begin{align*}
\lambda_a + \lambda_b & \rightarrow \lambda_{a+1} + \lambda_{b-1} & & \cdots & & \lambda_n + \lambda_{a+b-n} & & \cdots & & \lambda_{a+b-1} + \lambda_1 & & \lambda_{a+b} \\
\downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
\lambda_{a-1} + \lambda_{b-1} & \rightarrow \lambda_a + \lambda_{b-2} & & \cdots & & \lambda_{n-1} + \lambda_{a+b-n-1} & & \cdots & & \lambda_{a+b-2} \\
\vdots & & \vdots & & \vdots & & \vdots & & \vdots & & \vdots \\
\downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
\lambda_{n-b} + \lambda_{n-a} & \rightarrow \lambda_{n-b+1} + \lambda_{n-a-1} & & \cdots & & \lambda_{2n-a-b} \\
\vdots & & \vdots & & \vdots & & \vdots & & \vdots & & \vdots \\
\downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
\lambda_{a-b+1} + \lambda_1 & \rightarrow & & \lambda_{a-b+2} \\
\downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
\lambda_{a-b} & & & & & & & & & & 
\end{align*}$$

For $a + b > n$ the graph truncates at the $(n - a + 1)$th column, since the representations to the right of this column in the graph are then no longer present in the decomposition of $V_a \otimes V_b$. This fact will be crucial in examining the orders of the poles.
We must now decide the dependence of \( x(\theta, \beta) \) and \( q(\beta) \) on the rapidity difference \( \theta = \theta_1 - \theta_2 \) (where the incident particles’ rapidities are defined by \( p_i = (m_i \cosh \theta_i, m_i \sinh \theta_i) \) ) and on \( \beta \). For the \( d_{n+1}^{(2)} \) case, and in order to give the correct soliton mass ratios, we take

\[
x = e^{(n+1)\lambda \theta}, \quad \text{where} \quad \lambda = \frac{4\pi}{\beta^2} - \frac{2n}{n+1},
\]

and

\[
q = e^{i\omega \pi}, \quad \text{where} \quad \omega = \frac{2\pi}{\beta^2} - 1.
\]

In this paper we only discuss the case of generic \( q \) (i.e. \( q \) not a root of unity, equivalent to requiring that \( \omega \) not be rational). For other algebras, as discussed in [27], we need the forms given in appendix A, which are not yet properly understood. It is for this reason that we cannot yet give a derivation of the general \( S \)-matrix direct from the charge algebra, which we leave for future investigation.

## 2.1 Fusion and crossing properties

We now proceed with some results which we shall need later in fusing the \( S \)-matrices. First, we examine the fusion properties of the \( \tilde{R}(TPG) \). We are always free to rescale \( R \)-matrices by a scalar factor, and it turns out that the \( R \)-matrices preserved by fusion are not those given above, in which \( \tilde{P}_{\lambda_a+\lambda_b} \) has coefficient 1, but those for which \( \tilde{P}_{\lambda_a+\lambda_b} \) has coefficient 1. Denoting these \( R \)-matrices by \( \tilde{R}' \), we find

\[
\tilde{R}'_{a,b}(x) \equiv \prod_{j=1}^{a} \prod_{k=1}^{b} \left[ \tilde{R}'_{1,1}(xq^{-2-a-b+2j+2k}) \right]_{a+1-j,a+k}
\]

where the equation acts on \( V_a \otimes V_b \subset V_1^{\otimes(a+b)} \) and \( [ i,j \) indicates that the \( R \)-matrix is taken to act on the \( i \)th and \( j \)th \( V_1 \)s. The product is taken in order of increasing \( j \) and \( k \). The result holds because when \( x = q^{a+b} \) anti-symmetrization now takes place on all spaces, and \( \tilde{R}_{a,b} \) projects onto \( V_{a+b} \) with a coefficient which must, by unitarity, equal 1. This result still applies when the TPG is truncated.

Using

\[
\tilde{R}'_{a,b}(TPG)(x) = \prod_{k=1}^{b} -\langle a - b + 2k \rangle \tilde{R}'_{a,b}(x)
\]

we now obtain

\[
k_{a,b}(x)\tilde{R}'_{a,b}(TPG)(x) \equiv \prod_{j=1}^{a} \prod_{k=1}^{b} \left[ \tilde{R}'_{1,1}(xq^{-2-a-b+2j+2k}) \right]_{a+1-j,a+k}
\]
where
\[ k_{a,b}(x) = \prod_{l=1}^{b} \prod_{m=1}^{a-1} - (2l - 2m + a - b). \] (5)

The second result we need is an explicit formula for $R$-matrix crossing symmetry analogous to that conjectured to hold for the $a_n$ case in (3.16) of [28]. In appendix B we prove the result (55,56), which we now generalise to
\[ c_{a,b}(i\pi - \theta) \tilde{R}_{a,b}^{(TPG)}(x(i\pi - \theta)) = c_{a,b}(\theta) \tilde{R}_{a,b}^{(TPG)}(x(\theta)) \] (6)
in which
\[ c_{a,b}(\theta) = \prod_{k=1}^{b} \sin(\pi(\mu - \frac{\omega}{2}(a - b + 2k))) \sin(\pi(\mu - \frac{\omega}{2}(2n + 2 - a - b + 2k))) \] (7)
where
\[ \mu = -i \frac{(n+1)\lambda}{2\pi} \theta. \] (8)

The proof uses (4) and is equivalent to showing that the set of poles in the fused $\tilde{R}_{1,1}^{(TPG)}$, minus the set of poles in $\tilde{R}_{a,b}^{(TPG)}$ (including those which would appear in the truncated part of the TPG), is invariant under $\theta \mapsto i\pi - \theta$. (It should be noted that $c_{a,b}$ has zeros exactly where $\tilde{R}_{a,b}^{(TPG)}$ has poles.)

The last result is one we shall need in order to calculate the breather-soliton $S$-matrices in the next section,
\[ \tilde{R}_{a,b}^{(TPG)}(x(\theta)) = P_0 \otimes I_a \cdot I_b \otimes \tilde{R}_{a,b}^{(TPG)}(xq^{n+1}) \cdot \tilde{R}_{a,b}^{(TPG)}(xq^{-(n+1)}) \otimes I_b \]
\[ = \frac{c_{a,b}(\theta + \frac{i\pi}{2} - \frac{i\pi}{(n+1)\lambda})}{c_{a,b}(-\theta + \frac{i\pi}{2} - \frac{i\pi}{(n+1)\lambda})} \tilde{R}_{b,a}^{(TPG)}(x^{-1}q^{n+1}) \cdot \tilde{R}_{a,b}^{(TPG)}(xq^{-(n+1)}) \]
\[ = \prod_{k=1}^{b} \frac{\sin(\pi(\mu - \frac{\omega}{2}(a - b + 2k - n - 1))) \sin(\pi(\mu - \frac{\omega}{2}(n + 1 - a - b + 2k)))}{\sin(\pi(\mu + \frac{\omega}{2}(a - b + 2k - n - 1))) \sin(\pi(\mu + \frac{\omega}{2}(n + 1 - a - b + 2k)))} \times I_a. \] (9)
in which $I_a$ denotes the identity on $V_a$. This result is made most evident in the following diagram:
The first line acts on $V_a \otimes V_b \otimes V_b$, while the second acts on $V_a \otimes V_b$, with $\tilde{R}^{(TPG)}_{b,a}$ now acting in the crossed channel. Unitarity of the $R$-matrix then gives the third line, a simple scalar factor acting on $V_a$ in the direct channel.

3 Exact S-matrices for $d_{n+1}^{(2)}$ quantum affine Toda field theory

We now define the S-matrix for the scattering of elementary solitons to be

$$S_{a,b}(\theta) = F_{a,b}(\mu(\theta))k_{a,b}(\theta)\tau_{21}\tilde{R}^{(TPG)}_{a,b}(\theta)^{-1}$$

in which $\tau$ is the transformation from the homogeneous to the spin gradation described in appendix A, $k_{a,b}(\theta)$ is given by (5) and the overall scalar factor $F_{a,b}(\mu(\theta))$ will be constructed below.

3.1 Scalar factors

The scalar factors $F_{a,b}(\mu)$ have to be chosen such that the S-matrix $S_{a,b}(\theta)$ satisfies the axioms of exact S-matrix theory (for a more detailed account of the exact S-matrix axioms see, for instance, [14, 29, 30]). The two axioms which determine the scalar factor up to a so-called CDD-factor are the requirements of unitarity:

$$S_{a,b}(\theta)S_{b,a}(-\theta) = I_b \otimes I_a$$

and crossing symmetry:

$$S_{a,b}(\theta) = (I_b \otimes C_a)[\sigma S_{b,a}(i\pi - \theta)]t_2\sigma(C_\pi \otimes I_b) ,$$

in which $\tau$ is the transformation from the homogeneous to the spin gradation described in appendix A, $k_{a,b}(\theta)$ is given by (5) and the overall scalar factor $F_{a,b}(\mu(\theta))$ will be constructed below.
in which $\overline{a}$ represents the conjugate of $a$, $C_a$ is the charge conjugation operator, $t_2$ indicates transposition in the second space and $\sigma$ is the permutation operator. In the case of $d_{n+1}^{(2)}$ ATFT, in which all particles are self-conjugate, (12) reduces to

$$S_{a,b}(\theta) = [\sigma S_{b,a}(i\pi - \theta)]^{t_2}\sigma .$$

(13)

In the following we will use these equations to obtain the scalar factor $F_{1,1}$ in terms of products of gamma functions. In order to exploit the crossing symmetry requirement we need to examine the crossing symmetry properties of the R-matrix itself. As mentioned in section 2.1 we seek to find a scalar function $c_{1,1}(\theta)$ such that $c_{1,1}(\theta)\tilde{R}_{1,1}^{(TPG)}(\theta)$ is crossing symmetric, i.e. satisfies equation (11). By expressing the R-matrix in terms of the Birman-Wenzl-Murakami algebra [31, 32] we show in Appendix 3 that this function is given by

$$c_{1,1}(\theta) = \sin(\pi(\mu - \omega))\sin(\pi(\mu - (n + 1)\omega)) .$$

Writing $F_{1,1}(\mu(\theta)) = c_{1,1}(\theta)f_{1,1}(\mu(\theta))$ and using equation (12) for $a = b = 1$ (noting that $\mu(i\pi - \theta) = -\mu + \frac{n+1}{2}\lambda$) we obtain the first condition

$$f_{1,1}(-\mu + \frac{n+1}{2}\lambda) = f_{1,1}(\mu) .$$

(14)

Using $\langle l \rangle(\theta) = 1/\langle l \rangle(\theta)$ and the spectral decomposition of the R-matrix (3)

$$\tilde{R}_{1,1}^{(TPG)}(\theta) = \tilde{P}_{2\lambda_1} + \langle 2 \rangle\tilde{P}_{\lambda_2} + \langle 2n + 2 \rangle\tilde{P}_0$$

we can see immediately that

$$\tilde{R}_{1,1}^{(TPG)}(\theta)\tilde{R}_{1,1}^{(TPG)}(-\theta) = I_1 \otimes I_1 .$$

From this and equation (13) we obtain the second condition

$$f_{1,1}(\mu)f_{1,1}(-\mu) = c_{1,1}^{-1}(\theta)c_{1,1}^{-1}(-\theta) .$$

(15)

The standard method (see for instance [33, 34]) for solving (14) and (15) consists of choosing a suitable starting function $f^{(1)}(\mu)$, which satisfies equation (14), and multiplying it by a factor such that equation (15) is satisfied. Then equation (15) is violated again and one has to multiply this by another factor. Continuing this iteration process one ends up with

\footnote{The disagreement of this condition with equation (2.45) in [27] is due to the fact that Delius’ scalar factor is different from the one we use, since his factor $c_{1,1}$ is determined by the definition $\tilde{R}_{1,1}(\theta) = (\pi_1^{(0)} \otimes \pi_1^{(0)})R$ and is therefore not equal to our $c_{1,1}(\theta)$.}
an infinite product that satisfies both equations. The general solution to equations (14) and (15) is given by

\[ f_{1,1}(\mu) = \prod_{j=1}^{\infty} \frac{f^{(1)}[\mu + (n + 1)\lambda(j - 1)]f^{(1)}[-\mu + (n + 1)\lambda(j - \frac{1}{2})]}{f^{(1)}[\mu + (n + 1)\lambda(j - \frac{1}{2})]f^{(1)}[-\mu + (n + 1)\lambda j]} \]  

(16)

for any function \( f^{(1)}(\mu) \) with \( f^{(1)}(\mu)f^{(1)}(-\mu) = c_{1,1}^{-1}(\theta)c_{1,1}^{-1}(-\theta) \). In order to choose an appropriate starting function \( f^{(1)}(\mu) \) we rewrite

\[ c_{1,1}^{-1}(\theta)c_{1,1}^{-1}(-\theta) = \frac{1}{\pi^2}\Gamma(\mu - \omega)\Gamma(1 - \mu + \omega)\Gamma(\mu - (n + 1)\omega)\Gamma(1 - \mu + (n + 1)\omega) \]

\[ \times \Gamma(-\mu - \omega)\Gamma(1 + \mu + \omega)\Gamma(-\mu - (n + 1)\omega)\Gamma(1 + \mu + (n + 1)\omega). \]

For our purpose the only appropriate combination of gamma functions as a starting function is

\[ f^{(1)}(\mu) = \frac{1}{\pi^2}\Gamma(\mu - \omega)\Gamma(\mu - (n + 1)\omega)\Gamma(1 + \mu + \omega)\Gamma(1 + \mu + (n + 1)\omega). \]  

(17)

(Using any other combination will lead to a scalar factor with an infinite number of poles on the physical strip.) Using the solution (16) and \( \lambda = 2\omega + \frac{2}{\mu+1} \) we finally obtain the following scalar factor:

\[ F_{1,1}(\mu) = \prod_{j=1}^{\infty} \frac{\Gamma(\mu + (n + 1)\lambda j - \omega)\Gamma(\mu + (n + 1)\lambda j - (2n + 1)\omega - 1)}{\Gamma(-\mu + (n + 1)\lambda j - \omega)\Gamma(-\mu + (n + 1)\lambda j - (2n + 1)\omega - 1)} \]

\[ \times \frac{\Gamma(\mu + (n + 1)\lambda j - (n + 1)\omega)\Gamma(\mu + (n + 1)\lambda j - (n + 1)\omega - 1)}{\Gamma(-\mu + (n + 1)\lambda j - (n + 1)\omega)\Gamma(-\mu + (n + 1)\lambda j - (n + 1)\omega - 1)} \]

\[ \times \frac{\Gamma(-\mu + (n + 1)\lambda j - (n + 2)\omega - 1)\Gamma(-\mu + (n + 1)\lambda j - n\omega)}{\Gamma(\mu + (n + 1)\lambda j - (n + 2)\omega - 1)\Gamma(\mu + (n + 1)\lambda j - n\omega)} \]

\[ \times \frac{\Gamma(-\mu + (n + 1)\lambda j - 2(n + 1)\omega - 1)\Gamma(-\mu + (n + 1)\lambda j)}{\Gamma(\mu + (n + 1)\lambda j - 2(n + 1)\omega - 1)\Gamma(\mu + (n + 1)\lambda j)} . \]  

(18)

The bootstrap principle of exact S-matrix theory can be applied to obtain the general scalar factor \( F_{a,b}(\mu) \). We will show this in detail only for \( F_{2,1} \). After a careful study of the pole structure of \( S_{1,1}(\theta) \) it emerges that \( S_{1,1}(\theta) \) projects onto the module \( V_2 \) at the following poles (written in terms of \( \mu \) which was defined in (5)):

\[ \mu(\theta_p^{(2)}) = \omega - p \quad \text{(for } p = 0, 1, \ldots \leq \omega) \]

The lowest of these poles \( (p = 0) \) corresponds to the fusion process \( A^{(1)} + A^{(1)} \rightarrow A^{(2)} \) and from the bootstrap principle of analytic S-matrix theory we know

\[ S_{2,1}(\theta) = \left[ S_{1,1} \left( \theta + \frac{\theta_0^{(2)}}{2} \right) \right]_{1,3} \left[ S_{1,1} \left( \theta - \frac{\theta_0^{(2)}}{2} \right) \right]_{1,2} \]  

(19)
Since we also know from equation (4) that
\[ R_{1,1}^{(TPG)}(\theta + \frac{\theta_0^{(2)}}{2})_{1,2} \left[R_{1,1}^{(TPG)}(\theta - \frac{\theta_0^{(2)}}{2})\right]_{1,3} = k_{2,1}(\theta) R_{2,1}^{(TPG)}(\theta) \] we obtain the result:
\[ F_{2,1}(\mu) = F_{1,1}(\mu + \frac{\omega}{2}) F_{1,1}(\mu - \frac{\omega}{2}) . \]
Continuing this fusion procedure we find in general that the pole at
\[ \mu(\theta_0^{(a+b)}) = \frac{a + b}{2} \omega \] corresponds to the fusion process \( A^{(a)} + A^{(b)} = A^{(a+b)} \) of fundamental solitons and therefore we obtain the following expression for the general scalar factor:
\[ F_{a,b}(\mu) = \prod_{j=1}^{a} \prod_{k=1}^{b} F_{1,1}(\mu + \frac{\omega}{2}(2j + 2k - a - b - 2)) . \quad (21) \]

### 3.2 Soliton masses

We conjecture that the S-matrix defined in (10) describes the scattering of solitons in \( d_{n+1}^{(2)} \) ATFT. We explain how we expect the direct channel simple poles to match the soliton masses for general algebras in appendix A; here we point out that the lowest poles (20) which are at \( x(\theta_0^{(a+b)}) = a^{a+b} \) match precisely the soliton mass ratios calculated in [10]. We will demonstrate this briefly. We know that the classical soliton masses for \( d_{n+1}^{(2)} \) ATFT (in which \( h = n + 1 \) are given by
\[ M_a^{Cl} = 8\sqrt{2}\frac{hm}{\beta^2} \sin \left( \frac{a\pi}{2h} \right) . \quad (22) \]
Via the usual mass relation
\[ M_{a+b}^2 = M_a^2 + M_b^2 + 2M_aM_b \cosh(\theta_0^{(a+b)}) \] the poles (20) determine the quantum soliton masses (up to an overall scale factor \( C \)) to be
\[ M_a = C8\sqrt{2}\frac{hm}{\beta^2} \sin \left( \frac{a\pi}{h} \left( \frac{1}{2} - \frac{1}{h\lambda} \right) \right) . \quad (24) \]
Expanding this in terms of \( \beta^2 \) we obtain
\[ M_a = C8\sqrt{2}\frac{hm}{\beta^2} \sin \left( \frac{a\pi}{2h} \right) \left[ 1 - \beta^2 \frac{a}{4h^2} \cot \left( \frac{a\pi}{2h} \right) \right] + O(\beta^2) \]
which coincides with the result in [10] (table 4) provided that

\[ C = 1 + \frac{\beta^2}{8h} \cot \left( \frac{\pi}{2h} \right) \frac{1}{4\pi} h + O(\beta^4) \]

\[ = \frac{\beta^2}{4\pi \lambda} + \frac{\beta^2}{8h} \cot \left( \frac{\pi}{2h} \right) + O(\beta^4). \quad (25) \]

(It is not yet clear to us why the scale factor \( C \) should have this form.) We can also see that (up to an overall scale factor) the change from the classical to the quantum masses corresponds to a shift of the Coxeter number \( h \) to a so-called quantum Coxeter number:

\[ h \rightarrow h + \frac{1}{\omega}. \]

This is similar to the situation in real ATFT [21] and has also been pointed out in [27]. For a general discussion see appendix A.

We also should remark on the fact that our conjecture of the soliton S-matrix does not contain any additional CDD factors. In [14] a minimal Toda factor was necessary for the construction of a consistent S-matrix for \( a_n^{(1)} \) affine Toda solitons. In the case of non-simply laced ATFTs minimal (coupling constant independent) S-matrices do not exist (see [21]). However, we will see in the following sections that the scalar factor defined above already contains all the poles and zeros on the physical strip (i.e. \( 0 \leq \text{Im}(\theta) \leq \pi \)) necessary to satisfy the bootstrap equations, and we do not need to include any additional CDD factor. In the following sections we will further justify this conjecture by comparing the S-matrix elements of scalar bound states with the results in real ATFT and describing the pole structure in more detail.

### 3.3 Breather S-matrices

By applying the fusion procedure (or bootstrap method) in this section we construct the S-matrix elements for the scattering of bound states. Here this procedure is applied directly to the full S-matrix \( S_{a,b}(\theta) : V_a \otimes V_b \rightarrow V_b \otimes V_a \), whereas in [18] the same method has been applied to the scattering amplitudes (which are just scalar functions) of single solitons by using the Zamolodchikov algebra formalism.

Projectors onto singlets, which correspond to scalar bound states of elementary solitons, only appear in the elements \( \tilde{R}_{a,a}^{(TPG)} \) for \( a = 1, 2, \ldots, n \). We will call these scalar bound states ‘breathers’ and denote them by \( B_p^{(a)} \). The poles corresponding to these breathers must be
in the prefactor $\langle 2n + 2 \rangle$, since this is the factor which in the spectral decomposition (4) appears in front of $\hat{P}_0$ exclusively. $\langle 2n + 2 \rangle$ has the following poles on the physical strip:

$$\mu = (n+1)\omega + 1 - p \quad \text{for } p = 1, 2, \ldots \leq (n+1)\omega + 1.$$  \hfill (26)

At these values of the rapidity the S-matrix projects onto the module of the singlet representation and therefore the poles correspond to breather states with masses

$$m_{B_2}^{(p)} = 2M_a \sin \left( \frac{p\pi}{(n+1)\lambda} \right),$$

in which $M_a$ are the quantum masses of the fundamental solitons, given in (24).

The pole corresponding to the lowest breather (the bound state with lowest mass) is $\mu = (n+1)\omega$, which corresponds to $\theta = i\pi(1 - \frac{2}{(n+1)\lambda})$. Therefore we are able to obtain the S-matrix element for the scattering of a lowest breather of species $b$ with a fundamental soliton of species $a$ via the following bootstrap equation:

$$S_{A(a)B_1(b)}(\theta) \times I_a = I_b \otimes S_{a,b}(\theta + i\pi(\frac{1}{2} - \frac{1}{(n+1)\lambda})) \cdot S_{a,b}(\theta - i\pi(\frac{1}{2} - \frac{1}{(n+1)\lambda})) \otimes I_b.$$  \hfill (27)

Thus we need the following formula, derived in appendix C:

$$F_{a,b}(\mu + \frac{n+1}{2} - \omega) \times F_{a,b}(\mu - \frac{n+1}{2} - \omega) = \prod_{k=1}^b \frac{\sin(\pi(\mu + \frac{\omega}{2}(2k - a - b - 1 - n))) \sin(\pi(\mu + \frac{\omega}{2}(2k + a - b - 1 + n)))}{\sin(\pi(\mu + \frac{\omega}{2}(2k - a - b - 1 - n))) \sin(\pi(\mu + \frac{\omega}{2}(2k + a - b - 1 + n)))} \times \left( \frac{\omega}{2}(2k + a - b - 1 - n) \right) \left( \frac{\omega}{2}(2k - a - b - 1 - n) + 1 \right) \times \left( \frac{\omega}{2}(2k - a - b - 1 + n) \right) \left( \frac{\omega}{2}(2k - a - b + 1 + n) + 1 \right),$$  \hfill (27)

in which we have used the notation

$$y = \frac{\sin(\frac{\pi}{(n+1)\lambda}(\mu + y))}{\sin(\frac{\pi}{(n+1)\lambda}(\mu - y))}. \hfill (28)$$

Combining this with (3,14) we obtain the S-matrix element $S_{A(a)B_1(b)}$ for the scattering of an elementary soliton of species $a$ with a breather $B_1(b)$:

$$S_{A(a)B_1(b)}(\theta) = \prod_{k=1}^b \left( \frac{\omega}{2}(2k + a - b - 1 - n) \right) \left( \frac{\omega}{2}(2k - a - b - 1 - n) + 1 \right) \times \left( \frac{\omega}{2}(2k + a - b - 1 + n) \right) \left( \frac{\omega}{2}(2k - a - b + 1 + n) + 1 \right).$$  \hfill (29)
This can be written in a compact form by introducing the crossing symmetric blocks

\[ \{y\} \equiv (y)(n\omega + \omega + 1 - y)(y + n\omega)(w + 1 - y), \tag{30} \]

which have the following properties. They are crossing symmetric

\[ \{y\}_{\theta \to -i\pi - \theta} = \{(n + 1)\omega + 1 - y\} = \{y\} \]

and 2\(\pi\) periodic

\[ \{y\}_{\theta \to \theta + 2\pi i} = \{y + 2(n + 1)\omega + 2\} = \{y\}. \]

Therefore we can write

\[ S_{A^{(a)}B_1^{(b)}}(\theta) = \prod_{k=1}^{b} \left\{ \frac{\omega}{2} (a + b - 2k + 1 - n) \right\}. \tag{31} \]

This S-matrix element is just a scalar function which gives the scattering amplitude for the scattering of a fundamental soliton with a breather. This can formally be written as a braiding relation:

\[ A^{(a),j}(\theta_1)B_1^{(b)}(\theta_2) = S_{A^{(a)}B_1^{(b)}}(\theta_1 - \theta_2)B_1^{(b)}(\theta_2)A^{(a),j}(\theta_1), \tag{32} \]

in which the superscript \(j\) denotes the \(j\)th soliton in the \(a\)th multiplet. Since we will make no further use of relations of this kind, we will always omit the superscript \(j\). (For further details on this Zamolodchikov algebra see for instance [35] or [18]).

From (31) we obtain the breather-breather S-matrix by applying the same fusion procedure again:

\[ S_{B_1^{(a)}B_1^{(b)}}(\theta) = S_{A^{(a)}B_1^{(b)}}(\mu + \frac{n + 1}{2}\omega)S_{A^{(a)}B_1^{(b)}}(\mu - \frac{n + 1}{2}\omega) = \]

\[ = \prod_{k=1}^{b} \left( \frac{\omega}{2} (2k - 2 + a - b) \right) \left( \frac{\omega}{2} (2k + a - b) \right) \]

\[ \times \left( \frac{\omega}{2} (2n + 2k - a - b + 1) \right) \left( \frac{\omega}{2} (2n + 2k + 2 - a - b + 1) \right) \]

\[ \times \left( \frac{\omega}{2} (2k - a - b + 1) \right) \left( \frac{\omega}{2} (2k - 2 - a - b - 1) \right) \]

\[ \times \left( \frac{\omega}{2} (2n + 2k + 2 + a - b) + 2 \right) \left( \frac{\omega}{2} (2n + 2k + a - b) \right) = \]

\[ = \prod_{k=1}^{b} \left\{ \frac{\omega}{2} (a + b - 2k - 2n) \right\} \left\{ \frac{\omega}{2} (a + b - 2k + 2) \right\}. \tag{33} \]
Now we want to compare this expression with the S-matrix for the fundamental quantum particles, which was found in [21] for the real $d_{n+1}^{(2)}$ ATFTs:

\[
S_{ab}^{(r)}(\theta) = \prod_{k=1}^{b} \left\{ \frac{2k + a - b - 1}{2k + a + b + 1} \right\}_H \left( H - 2k - a + b + 1 \right)_H
\]

in which

\[
\{y\}_H = \frac{(y - 1)_H(y + 1)_H}{(y + B)_H(y + 1 - B)_H} \quad \text{and} \quad (y)_H = \frac{\sin(\frac{\theta}{2} + \frac{y\pi}{2H})}{\sin(\frac{\theta}{2} - \frac{y\pi}{2H})}.
\]

$H$ is twice the quantum Coxeter number, $H = 2n + 2 - 2B$ and we assume that the coupling constant dependent function $B$ is given by $B(\beta) = \frac{\beta^2}{2\pi + \beta}$ (cf [21] and [36], with appropriate normalisations). After analytic continuation ($\beta \to i\beta$) we are able to make the following identifications:

\[
H \to (n + 1) \frac{\lambda}{\omega}, \quad B \to -\frac{1}{\omega}, \quad \left( y \right)_H \rightarrow \left( \frac{\omega}{2}\right)_y.
\]

Applying this in (34) it finally emerges that:

\[
S_{ab}^{(r)}(\theta) \to S_{B_1^{(a)}B_1^{(b)}}(\theta).
\]

Thus $S_{B_1^{(a)}B_1^{(b)}}(\theta)$ is indeed identical to $S_{ab}^{(r)}(\theta)$ after analytic continuation ($\beta \to i\beta$) and we can therefore identify the lowest breather states $B_1^{(a)}$ with the $a$th fundamental quantum particle of the theory. This generalises results found for sine-Gordon and $a_2^{(1)}$-ATFT ([18]). Since there remains little doubt that the S-matrix for real ATFT found in [21] is correct this exact agreement with the lowest breather S-matrix provides the best possible justification so far for our S-matrix conjecture.

For completeness we also give the S-matrix elements involving higher breathers. These were constructed in the same way as shown for $B_1^{(a)}$ and can all be written conveniently in terms of the blocks $\{y\}_H$. We obtain the S-matrix elements for the scattering of a fundamental soliton $A^{(a)}$ with a breather $B_p^{(b)}$:

\[
S_{A^{(a)}B_p^{(b)}}(\theta) = \prod_{l=1}^{p} \prod_{k=1}^{b} \left\{ \frac{\omega}{2} (a + b - 2k + 1 - n) - l + \frac{1}{2} + \frac{p}{2} \right\},
\]

\[\text{For the S-matrix elements involving higher breathers we were not able to find a generalisation of the blocks } \{y\}_H \text{ used in real affine Toda theory, and it is for this reason that our definition of the blocks } \{y\} \text{ is not related to the blocks } \{y\}_H .\]
of two breathers $B_r^{(a)}$ and $B_p^{(b)}$

$$S_{B_r^{(a)}B_p^{(b)}}(\theta) = \prod_{l=1}^{p} \prod_{k=1}^{b} \left\{ \frac{\omega}{2} (a + b - 2k - 2n) - l + \frac{p + r}{2} \right\} \left\{ \frac{\omega}{2} (a + b + 2k + 2) + l - \frac{p + r}{2} \right\}$$ (37)

and of an excited soliton $A_r^{(2a)}$ (which will be defined in the next section) with a breather $B_p^{(b)}$:

$$S_{A_r^{(2a)}B_p^{(b)}}(\theta) = \prod_{l=1}^{p} \prod_{k=1}^{b} \left\{ \frac{\omega}{2} (b - 2k - n + 1) - l + \frac{1}{2} + \frac{p + r}{2} \right\} \left\{ \frac{\omega}{2} (2a + b - 2k - n + 1) + l - \frac{1}{2} - \frac{p + r}{2} \right\}.$$ (38)

The same fusion procedure could also be applied in order to construct the S-matrix for the scattering of two excited solitons. This S-matrix would not be just a scalar function, but, like $S^{a,b}(\theta)$, an intertwiner on the tensor product of the two corresponding modules. This construction, however, remains beyond the scope of this paper.

4 Pole structure

In this section we discuss the pole structure of our conjectured S-matrix. For the S-matrix to be consistent with the bootstrap equations we would need to explain its entire pole structure and show that the bootstrap closes on it. We show explicitly for the case of $d_3^{(2)}$ ATFT how all poles in the soliton S-matrix can be explained by fusion into bound states or by higher order diagrams. We also give some examples of how to explain poles in the bound state S-matrices. We will see that all important properties of the general theory already appear in the $d_3^{(2)}$ case and this will therefore lead us to conjecture the full spectrum of solitons and bound states and a complete set of three-point couplings in $d_{n+1}^{(2)}$ ATFT.
4.1 Example: $d_3^{(2)}$ ATFT

Before we study the pole structure of the general case in the next section, we provide here for the sake of clarity a detailed account of all the poles in the S-matrices for $d_3^{(2)}$. The notations defined in (3) reduce in the case of $n = 2$ to

$$\lambda = \frac{4\pi}{\beta^2} - \frac{4}{3}, \quad \omega = \frac{2\pi}{\beta^2} - 1$$

and thus $2\omega = \lambda - \frac{4}{3}$.

The S-matrix elements for the scattering of fundamental solitons can be written as

$$S_{1,1}(\theta) = F_{1,1}(\mu) \tau \{ \hat{P}_{2\lambda_1} + \langle 2 \rangle \hat{P}_{\lambda_2} + \langle 6 \rangle \hat{P}_0 \} \tau^{-1}$$

$$S_{2,1}(\theta) = -F_{2,1}(\mu) \langle 1 \rangle \tau \{ \hat{P}_{\lambda_1 + \lambda_2} + \langle 5 \rangle \hat{P}_{\lambda_1} \} \tau^{-1}$$

$$S_{2,2}(\theta) = F_{2,2}(\mu) \langle 0 \rangle \langle 2 \rangle \tau \{ \hat{P}_{2\lambda_2} + \langle 4 \rangle \hat{P}_{2\lambda_1} + \langle 4 \rangle \langle 6 \rangle \hat{P}_0 \} \tau^{-1}$$

(40)

(where we omit the indices from $\tau$). Using the expression (21) one can write down explicit expressions for the scalar factors in terms of gamma functions. After a careful study of their pole structure and taking all pole-zero cancellations into account we obtain the following simple poles on the physical strip. (For the sake of simplicity we will write the poles in terms of $\mu = -i\frac{3\lambda}{2\pi}\theta$, such that the physical strip corresponds to $0 \leq \text{Re}\mu \leq \frac{3}{2}\lambda = 3\omega + 1$ and $\text{Im}\mu = 0$.)

In $S_{1,1}(\theta)$:

$$\mu = \omega - p \quad \text{(for } p = 0, 1, 2, \ldots \leq \omega)$$

$$\mu = 3\omega + 1 - p \quad \text{(for } p = 1, 2, \ldots \leq 3\omega + 1)$$

(41)

and their cross channel poles:

$$\mu = 2\omega + 1 + p \quad \text{(for } p = 0, 1, 2, \ldots \leq \omega)$$

$$\mu = p \quad \text{(for } p = 1, 2, \ldots \leq 3\omega + 1).$$

In $S_{2,1}(\theta)$:

$$\mu = \frac{5}{2}\omega + 1 - p \quad \text{(for } p = 0, 1, 2, \ldots \leq \frac{5}{2}\omega + 1)$$

(42)

and their cross channel poles:

$$\mu = \frac{1}{2}\omega + p \quad \text{(for } p = 0, 1, 2, \ldots \leq \frac{5}{2}\omega + 1).$$
In $S_{2,2}(\theta)$:

\[
\begin{align*}
\mu &= 2\omega + 1 - p & (\text{for } p = 0, 1, 2, \ldots \leq 2\omega + 1) \\
\mu &= 3\omega + 1 - p & (\text{for } p = 1, 2, \ldots \leq 3\omega + 1)
\end{align*}
\]  

(43)

and their cross channel poles:

\[
\begin{align*}
\mu &= \omega + p & (\text{for } p = 0, 1, 2, \ldots \leq 2\omega + 1) \\
\mu &= p & (\text{for } p = 1, 2, \ldots \leq 3\omega + 1).
\end{align*}
\]

Now we will try to explain all these poles either by fusion processes or higher order scattering diagrams. As already mentioned in the previous section the poles $\mu = 3\omega + 1 - p$ in $S_{1,1}(\theta)$ and in $S_{2,2}(\theta)$ appear in front of the projectors onto the singlet representations and are therefore expected to correspond to scalar bound states $B_p^{(1)}$ and $B_p^{(2)}$ (for $p = 1, 2, \ldots \leq 3\omega + 1$) with masses determined by the mass formula (23).

The second set of poles in $S_{1,1}(\theta)$ can be identified as the poles corresponding to bound states transforming under the module $V_2$. We will call these bound states excited solitons of type 2 and denote them as $A_p^{(2)}(\theta)$. The term ‘excited soliton’ was chosen in order to highlight the fact that the state with $p = 0$ is indeed just the fundamental soliton $A^{(2)}$.

In the light of this last definition one is tempted to identify the poles in $S_{2,1}(\theta)$ as corresponding to some sort of excited solitons transforming under $V_1$, in particular since the lowest pole $\mu = \frac{5}{2}\omega + 1$ indeed corresponds to the fusion $A^{(1)} + A^{(2)} \rightarrow A^{(1)}$. However, closer examination reveals that for $p \geq 1$ these poles cannot be explained by fusion into bound states. They do not take part in the bootstrap and one has to find a different interpretation. We will find that they can be explained by a subtle generalisation of a mechanism first discovered in the sine-Gordon theory by Coleman and Thun in [37]. The simplest example for such a generalised Coleman-Thun mechanism is a crossed box diagram, in which the scattering element in the middle displays a zero such that the expected double pole from the diagram is reduced to a simple pole. This mechanism was first described in [38] in connection with the $S$-matrices of nonsimply laced real ATFTs and has also been applied in [25] and in imaginary $a_2^{(1)}$ ATFT [18] to explain several simple poles in the $S$-matrix elements. Figure 1 shows such a crossed box diagram which indeed corresponds exactly to those poles in $S_{2,1}(\theta)$ which we are trying to explain. If all particles in a diagram like figure 1 are on shell then the angles (which correspond to purely imaginary rapidity
differences) in the diagram are fixed uniquely and can be calculated by using elementary geometrical considerations. In figure 1 we obtain the rapidity difference of the incoming particles to be $\mu = \frac{\omega}{2} + p$ in which $p = 1, 2, \ldots \leq \frac{5}{2} \omega + 1$. Since we also find that the internal scattering process occurs at $\mu = \frac{5}{2} \omega + \frac{p}{2} + \frac{1}{2}$, at which $S_{A^{(i)}B^{(j)}}$ displays a simple zero, we have shown that the diagram in figure 1 explains all remaining poles in $S_{1,2}(\theta)$.

![Figure 1](image)

(In this and all following diagrams time is moving upwards.)

The only set of poles not explained so far are the poles $\mu = 2w + 1 - p$ in $S_{2,2}(\theta)$. The lowest one of these poles ($p = 0$) is explained by another crossed box diagram, this time with $A^{(2)}$ on all the external and $A^{(1)}$ on all the internal legs (see figure 2). Here we encounter a slight variation of the generalised Coleman-Thun mechanism first pointed out by Hollowood [25]. This diagram again gives a naive double pole, and here the internal $S$-matrix element is non-zero. That the diagram nevertheless corresponds to a simple pole is owing to the fact that, although non-zero, the internal $S_{1,1}$ projects onto $V_2$, which is not present in the external legs’ $V_2 \otimes V_2$ because of truncation of the TPG. This mechanism generalises to all the non-particle $p = 0$ poles and is explained in appendix [3], where it is also used to explain the rational $S$-matrix pole structure.
The rest of the poles (for $p > 0$), however, correspond to an even more complicated generalised Coleman-Thun mechanism depicted in figure 3. In this diagram we find the rapidity difference of the two incoming particles $A^{(2)}$ to be $\mu = 2\omega + 1 - p$ in which $p$ can take values $1, 2, ..., \leq 2\omega + 1$. These are exactly the poles in $S_{2,2}(\theta)$ which we are trying to explain. However, the diagram in figure 3 contains five loops and thirteen internal lines and should therefore lead to cubic poles. The black dots in the diagram represent scattering processes of the internal particles. Calculating the internal angles of the diagram it emerges that the internal $A^{(1)} - A^{(1)}$ scattering process occurs at the rapidity difference $\mu = \omega + 1 - p$ at which $S_{1,1}(\theta)$ has neither pole nor zero. The two $B^{(1)} - A^{(1)}$ processes, however, occur at a rapidity difference of $\mu = \omega + 1 - \frac{p}{2}$ and from (31) we can see that at exactly those values $S_{A^{(1)}B^{(1)}}(\theta)$ displays a simple zero, which reduces the expected cubic pole to the observed simple poles in $S_{2,2}(\theta)$. 

Figure 2

Figure 3
The pole structure of the S-matrix lead us to conjecture the following particle spectrum of $d_3^{(2)}$ ATFT:

1) *fundamental solitons* $A^{(a)}$ ($a = 1, 2$):
   
   masses $M_a = C8\sqrt{2m_0} \sin(\frac{4\pi}{3}(\frac{1}{2} - \frac{1}{3\lambda}))$

2) *breathers* $B^{(a)}_p$ ($A^{(a)} - A^{(a)}$ bound states) ($a = 1, 2$ and $p = 1, 2, \ldots \leq 3\omega + 1$):
   
   masses $m_{B^{(a)}_p} = 2M_a \sin(\frac{2\pi}{3\lambda})$

3) *breathing solitons* $A^{(2)}_p$ ($A^{(1)} - A^{(1)}$ bound states) ($p = 0, 1, 2, \ldots \leq \omega$)
   
   masses $m_{A^{(2)}_p} = 2M_1 \cos(\frac{\pi}{6} - \frac{\pi}{9\lambda} - \frac{\pi p}{3\lambda})$.

Here we should mention a problem that occurred in [9]. Hollowood rejected his $c_n$ invariant S-matrix because there was a pole at $\theta = i\frac{\pi}{2}$ in $S_{a,n+1-a}$ which could not be explained in terms of the particle spectrum of the theory. Here we can see that in the weak coupling limit ($\lambda \to \infty$) the element $S_{2,1}$ has poles only at $\theta = i\frac{5\pi}{6}$ and $i\frac{\pi}{6}$. So due to the definitions (3) and the fact that we do not need to include an additional minimal Toda factor, the poles, which caused serious problems in [25], do not appear in our S-matrix conjecture.

We expect that it will prove possible to explain all poles in the S-matrix elements involving breathers in a similar way. We will show this for one example, the scattering of the two breathers $B^{(1)}_r$ and $B^{(1)}_p$. Without loss of generality we choose $r \geq p$. The S-matrix element $S_{B^{(1)}_r B^{(1)}_p}(\theta)$ was given in (37) and in the case of $n = 2$ contains the following simple and double poles on the physical strip:

$$
\mu^{(1)}_l = \omega - l + 1 - \frac{r - p}{2}
$$

$$
\mu^{(2)}_l = 2\omega + l + \frac{r - p}{2} \quad \text{(simple poles for } l = 1, 2, \ldots, p)\n$$

and

$$
\mu^{(3)}_l = 3\omega + l + 1 - \frac{r + p}{2}
$$

$$
\mu^{(4)}_l = -l + \frac{r + p}{2} \quad \text{(double poles if } l = 1, 2, \ldots, p - 1; \text{ simple poles if } l = 0, p) .
$$

By using the mass formula (23) we obtain that two breathers can fuse together to build another breather only if either the species or the excitation numbers of the two incoming breathers are identical. Thus in general the only possible fusion processes of two breathers are $B^{(a)}_r + B^{(a)}_p \to B^{(a)}_{r\pm p}$ and $B^{(a)}_p + B^{(b)}_p \to B^{(a+b)}_p$ (see section 4.2, figure 5d and 5e).
Therefore in our example we have two possible fusion processes, i.e. \( B_r^{(1)} + B_p^{(1)} \rightarrow B_{r\pm p}^{(1)} \), which explain the simple poles \( \mu_l^{(3)} \) and \( \mu_l^{(4)} \) for \( l = 0, p \).

The double poles \( \mu_l^{(3)} \) and \( \mu_l^{(4)} \) are the direct and cross channel poles corresponding to the crossed box diagram in figure 4a. Unlike in the case of figure 1, the process in the centre of the diagram occurs at a rapidity difference where the corresponding S-matrix has neither pole nor zero, and therefore the process in figure 4a leads to a double pole.

In order to explain the remaining poles \( \mu_l^{(1)} \) and \( \mu_l^{(2)} \) we find another third order diagram, depicted in figure 4b (in which \( s \) can take values \( s = 1, 2, ..., p \)). Here again two of the three internal scattering processes display a simple zero, which reduces the expected triple poles to simple poles.

In the following section we will extend this discussion to the general case of \( d_{n+1}^{(2)} \) ATFT.

### 4.2 \( d_{n+1}^{(2)} \) ATFT

From our observations in the \( d_{3}^{(2)} \) case we are able to conjecture the following particle spectrum for imaginary \( d_{n+1}^{(2)} \) ATFT:

1) **fundamental solitons** \( A^{(a)} \) \( (a = 1, 2, ..., n) \):

masses \( M_a = C8\sqrt{2}^{(n+1)m}\frac{m}{\beta^2} \sin\left(\frac{\alpha \pi}{n+1} \left( \frac{1}{2} - \frac{1}{(n+1)\lambda} \right) \right) \)
2) *breathers* $B_p^{(a)}$ ($A^{(a)} - A^{(a)}$ bound states) ($a = 1, 2, ..., n$ and $p = 1, 2, ..., \leq (n + 1)\omega + 1$):

masses $m_{B_p^{(a)}} = 2M_a \sin \left( \frac{p\pi}{(n+1)\lambda} \right)$

3) *breathing solitons* $A_p^{(2a)}$ ($A^{(a)} - A^{(a)}$ bound states) ($p = 0, 1, 2, ..., \leq a\omega$)

masses $m_{A_p^{(2a)}} = 2M_a \cos \left( \frac{p \pi}{n+1} \left( \frac{1}{2} - \frac{1}{(n+1)\lambda} - \frac{p}{a\lambda} \right) \right)$.

We have not examined the full pole structure of all S-matrix elements explicitly. Generalising the results of the $d_3^{(2)}$ case, however, we conjecture a list of all possible three point vertices in the theory. These six vertices seem to be the only vertices which are consistent with the mass formula (23) and the pole structure of the S-matrix. Although we are not able to give a general proof that this list is complete, all poles and diagrams we were able to examine could be explained by using only these vertices. (In the diagrams we have used the abbreviation $\tilde{\mu} \equiv \mu(i\pi) = (n + 1)\omega + 1$):

![Diagrams](image-url)

Figure 5a  
Figure 5b  
Figure 5c

Figure 5d  
Figure 5e  
Figure 5f

Due to the bootstrap principle all fusion processes obtained by turning any of the above diagrams by 120 degrees are also possible. It might seem a surprise that there are only
excitations of solitons of even species (figure 5c). However, in \[3\] the bound states of the classical soliton solutions of \(a_n^{(1)}\) ATFTs were studied and it was found that only solitons of species \(2\equiv h\) can be excited. Since the ‘\(\text{mod} h\)’ results from non-self-conjugacy of the representations of the \(a_n\) algebras, we expect that for \(d_{n+1}^{(2)}\) algebras (even in the classical case) excited solitons exist for even species only.

It should also be noted that, as already discovered in the \(a_2^{(1)}\) case \([18]\) and for the classical solitons of \(a_n^{(1)}\) AFTF \([3]\), only fundamental solitons of the same species (and of conjugate species in non-self-conjugate theories) can form bound states (figures 5b and 5c). We expect this to be a common feature of all imaginary ATFTs.

\section{Discussion}

In this paper we have demonstrated how to construct consistent soliton S-matrices for \(d_{n+1}^{(2)}\) affine Toda field theories by using trigonometric solutions of the Yang-Baxter equation, previously only carried out successfully for \(a_n^{(1)}\) ATFTs. The crux of the extension to nonsimply-laced algebras is the fact that the mass ratios of the solitons change under renormalisation. This is accommodated by changing the dependence of the spectral parameter \(x\) and the deformation parameter \(q\) on the physical variables \(\beta^2\) and \(\theta\) in equation (3) (see also \([19, 27, 33, 40]\)). After finding an appropriate overall scalar factor we constructed the S-matrices for all scattering processes involving breathers, and we were able to show that the S-matrix of the lowest breather states coincides with the exact S-matrix for the fundamental quantum particles (35). This identification has so far only been shown for sine-Gordon theory and in the case of \(a_2^{(1)}\). Because of the self-conjugacy of \(d_{n+1}^{(2)}\) ATFT the calculations in this paper were slightly easier than in the case of \(a_n^{(1)}\) theory. However, we have obtained some preliminary results in demonstrating the particle-breather identification for \(a_n^{(1)}\) ATFT which will appear in a forthcoming paper.

\subsection{Duality}

There are two ways in which these theories might exhibit some form of duality: affine duality, in which the weak regime of the \(\hat{g}\) theory is related to the strong regime of the \(\hat{g}^{\vee}\) theory, and Lie duality, in which objects in the \(g^{(1)}\) theory are related to others in the \(g^{(1)\vee}\)
theory, probably in the same regime. We can examine the possibilities within the following scheme, which is intended only as a tentative framework for discussion:

\[
\begin{array}{c|c}
weak/strong & \leftrightarrow & strong/weak \\
g^{(1)} \text{ solitons} & \leftrightarrow & g^{(1)\vee} \text{ solitons} \\
g^{(1)} \text{ breathers} & \leftrightarrow & g^{(1)\vee} \text{ breathers} \\
g^{(1)} \text{ particles} & \leftrightarrow & g^{(1)\vee} \text{ particles} \\
U_q(g^{(1)\vee}) & \supset & U_q(g^{(1)}) \\
\end{array}
\]

where \(g^{(1)\vee}\) means \(((g^{\vee})^{(1)})^{\vee}\) and so on.

In this paper we have examined the right-hand column in the weak regime and identified the breathers with the particles. It is unclear whether a strong regime exists: as we pointed out in appendix [3], both \(\lambda\) and \(\omega\) become singular at finite \(\beta\), and breathers and excited solitons disappear from the spectrum. However, there is certainly affine duality between the particles on the right at coupling \(4\pi/i\beta\) and on the left at \(i\beta\) [13]. If we formally examine the soliton and breather masses on the right at \(4\pi/i\beta\) we find that the mass ratios are consistent with this scheme - i.e. are the same for all the objects - if both the coupling for solitons and breathers on the left is \(\beta\) and, as mentioned before, the soliton mass corrections on the left are as in the note to [10], a matter which still remains for us to clarify.

There is, therefore, a possible Lie duality between \((g^\vee, i\beta)\) particles and \((g, \beta)\) breathers, extendable to the original classical Lie duality [3] suggested between \(g\) solitons and \(g^\vee\) particles which would also apply in the quantum case between \((g, \beta)\) solitons and \((g^\vee, i\beta)\) particles [8]. For the solitons, a \textit{sine qua non} for affine duality is that the \(S\)-matrices should have the same algebraic structure. This is guaranteed by the observation in the last row: that not only \(g^\vee \subset g^{(1)\vee}\) but also \(g^\vee \subset g^{(1)\vee}\). In our example, \(g = b_n\) and \(g^{(1)\vee} = d^{(2)}_{n+1}\), and the observation is that, with the appropriate choice of affine root, \(c_n \subset d^{(2)}_{2n-1}\). However, it is then difficult to see in what sense the two charge algebras could be dual, although a mechanism might be provided by [11]. (Further, if the note in [12] is correct and the \(U_q(c_n)\)-invariant \(R\)-matrix which must be used to describe \(b^{(1)}_n\) solitons is obtained from that for the \(d^{(2)}_{n+1}\) solitons by setting \(q^{h'} \mapsto -q^{h'-2}\), it is difficult to see how the correct masses could be obtained. This is connected with the difficulties described in appendix [A] and which we hope to resolve in future work.)
Whereas in the particle case affine duality included identification of the $S$-matrices (possible since the particles have masses of order $m$ in both weak and strong regime), this cannot be so simple for the solitons, which, if they exist in the strong regime, will have light masses in contrast to their heavy masses (of order $m/\beta^2$) in the weak regime. As we point out in appendix [4], this manifests itself in an overall rescaling of $\lambda$ and $\omega$ in the strong regime which gives the correct soliton mass ratios but forbids the existence of excited states, and which makes the leading-order $R$-matrix structure of the $S$-matrix trivial. A possibility for incorporating Lie, affine and strong-weak duality might therefore be that between the $(g^{\psi (1)}, 4\pi/i\beta)$ solitons and the $(g^{\psi (1)}, i\beta)$ particles. This and other possible relations might be explored by truncating the theory to admit only soliton degrees of freedom and then examining the relations between the semiclassical limits of the soliton and particle $S$-matrices and the soliton time delay [13, 14, 11]. For clarity we illustrate the possibilities as they apply to our example, $g = b_n$:

\[
\begin{array}{c c c c}
\text{solitons} & \leftrightarrow & \text{solitons} \\
\updownarrow & & & \\
\text{breathers} & \leftrightarrow & \text{breathers} \\
\text{particles} & \leftrightarrow & \text{particles} \\
U_q(a_{2n-1}^{(2)}) & \supset & U_q(c_n) & \subset & U_q(c_{n}^{(1)})
\end{array}
\]

It will require much more work on the untwisted nonsimply-laced solitons and their $S$-matrices, however, to place such speculation on a firmer footing.

5.2 More open problems

We do not know a general method of determining which fusion processes are allowed and so cannot prove that the suggested list of three-point vertices in section 4.2 is complete. It would be interesting to investigate whether there is a way of obtaining all possible three-point vertices from the properties of the underlying quantum group symmetry. This could eventually lead to a generalisation of Dorey’s fusing rule [14], which for real ATFT connects the possible fusion processes with properties of the root system of the associated Lie algebra. (For recent work on this fusing rule as it applies to decomposition of tensor products of representations of quantized affine algebras and Yangians see [15].) In order to do this we will also need a better understanding of what conserved quantities distinguish
bound states of the same species. In particular, it seems important to understand the relationships between the commuting, local conserved charges of the particles \[15\] (which have spins equal to the exponents of the algebra), those of the solitons \[1\], and the non-commuting, non-local \(U_q(\hat{g}^\vee)\) charges. Finally, on a mathematical level we have no idea how the excitation level \(p\) is related to quantized affine algebra representations.

Another unsolved problem in the imaginary ATFTs is that of unitarity. The complexity of the Hamiltonian implies a non-unitary theory, but we nevertheless believe that some truncation to a unitary theory of the solitons and their bound states will prove possible \[11\]. The \(S\)-matrices we have constructed obey the usual two-particle real unitarity, but we have not been able to examine the residues of the poles in sufficient detail to investigate one-particle unitarity (a requirement if the bootstrap principle is to be implemented properly). An investigation of the residues of poles would also be necessary in order to obtain a general criterion for which simple poles take part in the bootstrap and which are explained by some generalised Coleman-Thun mechanism, a connection found for real ATFTs in \[38\].

As mentioned previously, it would also be interesting to check the consistency of our \(S\)-matrix conjecture with semiclassical calculations, as done for \(a_n^{(1)}\) in \[14\]. The extension of this in particular to untwisted theories might help us to clarify the semiclassical mass calculations of \[24\] and \[10\].

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### A S-matrix parameters for general algebras

In the table (in which for the moment we restrict ourselves to the classical series) we use the notation of [15, 10]. The Coxeter and dual Coxeter numbers of the algebra are $h$ and $h^\vee$, whilst the difference between them and the $h', h'^\vee$ is well-known (see e.g. [36]) to be incapable of absorption into a single overall convention; $t = \frac{h' h'^\vee}{h h^\vee}$. A general form for $x$ and $q$ which gives the correct soliton mass ratios is then

$$x(\theta) = e^{h \lambda \theta}, \quad q = e^{\omega i \pi},$$

with

$$\lambda = \frac{4 \pi}{\beta^2} - \frac{h^\vee}{h}, \quad \omega = \frac{h}{h'} \left( \frac{4 \pi}{\beta^2} - t \right).$$

The crossing parameter $x(i \pi)$ is expected to be $+q h'$ for algebras whose affine dual is untwisted, and $-q h'$ for those whose affine dual is twisted (see [12, 16]). This works fine for all except the $a^{(2)}$ series, where we obtain minus the expected value. This may be resolved by multiplying $\lambda$ and $\omega$ by 2, since neither crossing nor any other pole knows about the
scale of the exponent in $x$ and $q$ (this ambiguity is mentioned in [27]). However, such an ad hoc resolution is clearly unsatisfactory, particularly since the form (44) of $x$ is by now well-known [19, 47, 39, 40] and is due to the transformation from the physical ‘spin’ gradation to the homogeneous gradation, in which all the $\theta$-dependence is transferred to the step operator corresponding to $\alpha_0$, and in which the $R$-matrices (3) are written. This is the generalisation to the nonsimply-laced case of the redefinition of in-/out-states (relative to the quantum group representations) required in [18]. Specifically, there exist non-local charges which form $U_q(\hat{g}^{\vee})$ [19, 12, 39, 13] and which transform as

$$L_\theta(E_i^\pm) = e^{s_i\theta}E_i^\pm$$

where $s_i = \frac{8\pi}{\alpha_i^2\beta^2} - 1$

under the action of a Lorentz boost $L_\theta$. For any $y$ we now have

$$y^{h_i}E_i^{\pm'} y^{-h_i} = y^{\alpha_i,\alpha_j} x E_j^{\pm'}$$

(45)

where the $E_i^{\pm'}$ are step operators, and the $h_i$ Cartan subalgebra generators, in any gradation. If we do a similarity transformation on the (homogeneous gradation) $R$-matrix

$$R(x, q) \rightarrow \tau_{21} R(x, q) \tau_{12}^{-1} ,$$

where

$$\tau_{12} = y^{-h_i\alpha_i}(\theta_1) \otimes y^{-h_i\alpha_i}(\theta_2)$$

(for some unspecified $y(\theta)$), then we must solve

$$y^{\alpha_i,\alpha_j} a_j x^{\delta_{i0}} = e^{s_i\theta}$$

if we wish to obtain the homogeneous gradation. In fact we can solve for $x$ without needing to know $y$ or $a_j$ by taking the product of the $n_i$th powers of these equations (where $n_i$ are the Kac marks of $\hat{g}^{\vee}$), and then have

$$x = \exp\sum_{i=0}^{r} n_i \left(\frac{8\pi}{\beta^2\alpha_i^2} - 1\right) \theta$$

$$= \exp h\lambda\theta ,$$

where

$$\lambda = \left(\frac{4\pi}{\beta^2} - \frac{h^{\vee}}{h}\right) .$$

It is now clear how flexible pole structure occurs: for self-dual algebras, with $h = h^{\vee}$, the $\beta$-dependences of $x$ and $q$ are proportional, and the ‘base’ pole (corresponding to an
unexcited soliton) does not involve \( \beta \): masses do not renormalise. For the other algebras we have

\[
\theta_r = i\pi \frac{r}{h'} \left( 1 - \frac{\beta^2}{4\pi t} \right).
\]

(We write out \( \lambda \) and \( \omega \) explicitly each time for transparency.) If \( M_a \sim \sin \left( \frac{a\pi}{H} \right) \), the fusions \( a, b \to a \pm b \) at \( r = a \pm b \) (in the direct and crossed channels respectively) require

\[
H = h' \frac{1 - \frac{\beta^2}{4\pi h}}{1 - \frac{\beta^2}{4\pi t}}.
\]

This gives precisely the particle mass ratios: \( \text{i.e. if exact } S\text{-matrices exist in this form, the soliton mass ratios for nonsimply-laced untwisted algebras must be as in } [8] \text{ and the note to } [10].\]

We can interpolate between affine dual algebras in two ways: either by

\[
H = h' + \frac{h'}{h}(h - h') \frac{\beta^2}{4\pi t},
\]

or by

\[
\frac{1}{H} = \frac{1}{h'} \frac{1}{h} \left( \frac{h - h'}{h' - th} \right) \frac{\beta^2}{4\pi h}.
\]

(Note that this does not work so neatly if we try to interpolate \( h \) and \( h' \) rather than \( h' \) and \( h'' \).) Notice how duality might work: \( \beta \mapsto \frac{4\pi}{\beta} \) leads to

\[
H \mapsto h'' \frac{1 - \frac{\beta^2}{4\pi h}}{1 - \frac{\beta^2}{4\pi t}},
\]

so that \( g \mapsto g' \) (with \( (h, h') \mapsto (h', h) \) and \( t \mapsto 1/t \)). However, the exponents \( \lambda \) and \( \omega \) receive an overall factor \(-\beta^2/4\pi\), so that the \( S\)-matrix is fundamentally different (with, for example, no excited state poles); any duality must be much more subtle than that for the particles.

Now consider poles for breathers and excited solitons. The possibility of such objects arises because of the ambiguity in the above pole: \( x(\theta_p^{(a+b)}) = q^{a+b}e^{-2i\pi t} \) gives

\[
\theta_p^{(a+b)} = \frac{i\pi}{H} \left( a + b - \frac{2p}{\omega} \right)
\]

which gives, via the usual mass relation, physical poles for \( p = 1, 2, ... \leq \frac{1}{2}\omega(a + b) \), all transforming at the singular value of the \( R\)-matrix \( x = q^r \) and thus in the same particle.
multiplet. Of course, the possibility of such poles does not necessarily lead to their presence in the $S$-matrix, and, as we saw for $d_3^{(2)}$, such poles do not all correspond to excited solitons.

For scalar breathers we need $x(\theta_p^{(0)}) = q^p e^{-2p\pi \hbar} e^{-\left(\hbar \nu - \hbar \theta \right)i\pi}$. This occurs at

$$\theta_p^{(0)} = \frac{i\pi}{p} \left(1 - \frac{2p}{\hbar \lambda}\right),$$

so that if a parent soliton of mass $M_a$ has a pole at $i\pi$ in its self-interaction then it can have a spectrum of breathers with masses

$$m_p^{(a)} = 2M_a \sin \left(\frac{p\pi}{\hbar \lambda}\right) \quad \text{(for} \quad p = 1, 2, \ldots, \leq \frac{1}{2}\hbar \lambda). \quad (46)$$

Note that the running couplings $\lambda$ and $\omega$ become zero at $\beta^2 = 4\pi \frac{\hbar}{\hbar \nu}$ and $4\pi / t$ respectively, and the excited states disappear from the spectrum for large $\beta$. In the simply-laced cases, and by analogy with the sine-Gordon theory, these coincide to give a rational limit for the $R$-matrix and an expected Yangian symmetry as $\beta^2 \to 4\pi$. In the non-simply-laced theories, we do not have $x, q \to 1$ simultaneously. The nature of these limits should be studied: for example, at $\beta^2 = 4\pi / t$ we appear to have a trivial $S$-matrix and thus a free theory. Recall also that at the point at which the $n$th breather enters the spectrum the sine-Gordon $S$-matrix becomes reflectionless and equal to the $d_n^{(1)}$ real ATFT $S$-matrix [15]. It seems to us that all such special values of $\lambda$ and $\omega$ are potentially interesting and deserving of study.
B Crossing symmetry of $\tilde{R}_{1,1}$

In order to prove the crossing symmetry of the R-matrix we use the Birman-Wenzl-Murakami algebra $\mathfrak{B}$ in its diagrammatic notation (for details see $\mathfrak{B}$):

Identity $\equiv$ 

Monoid $\equiv$ 

Braid $\equiv$ 

$(\text{Braid})^{-1} \equiv$ 

These symbols can be multiplied simply by concatenation and they satisfy the following relations:

\[
\begin{align*}
\bigotimes - \bigotimes &= m \left( \bigotimes - \right) \\
\left( \bigotimes \right) \bigotimes &= l^{-1} \\
\bigotimes \left( \bigotimes \right) &= l \\
\end{align*}
\] 

(47) \hspace{1cm} (48)

in which $m = q - q^{-1}$ and $l = -q^{2n+1}$ in the case of $c_n^{(1)}$. Now we want to express the lowest R-matrix in terms of these symbols. We know from (2) that:

\[
\tilde{R}_{1,1}^{(TPG)}(\theta) = \tilde{P}_{2\lambda_1} + \langle 2 \rangle \tilde{P}_{2\lambda_2} + \langle 2n + 2 \rangle \tilde{P}_0 .
\] 

(49)

The projectors can be expressed in the following way $\mathfrak{B}$:

\[
\begin{align*}
\tilde{P}_{2\lambda_1} &= \frac{1}{1 + q^2} \left[ \bigotimes + q \bigotimes + \frac{q - q^{-1}}{q^{-1} + q^{2n+1}} \right] \\
\tilde{P}_{2\lambda_2} &= \frac{1}{1 + q^{-2}} \left[ \bigotimes - q^{-1} \bigotimes + \frac{(1 + q^{-2n-2})(q - q^{-1})}{(1 - q^{-2n})(q^{-1} + q^{2n+1})} \right] \\
\tilde{P}_0 &= -\frac{q - q^{-1}}{(1 - q^{-2n})(q^{-1} + q^{2n+1})} \\
\end{align*}
\] 

(50)

Using the expressions $\mathfrak{B}$ in the expression of $\tilde{R}_{1,1}^{(TPG)}$ we obtain after some algebra:

\[
\tilde{R}_{1,1}^{(TPG)}(\theta) = \frac{x(1 - q^2)}{x - q^2} \bigotimes + \frac{(x - 1)q}{x - q^2} \bigotimes + \frac{x(x - 1)(1 - q^2)}{(x - q^2)(q^{2n+2} - x)} \\
\] 

(51)
We want to calculate the crossed version of this R-matrix:

\[ \check{R}_{1,1}^{(TPG)\text{cross}}(i\pi - \theta) = [\sigma \check{R}_{1,1}^{(TPG)}(i\pi - \theta)]^{12}\sigma . \]

Now the reason for the use of the BWM algebra becomes clear, since under the change to the crossed version the generators of the BWM algebra are transformed simply by turning them through 90 degrees. This exchanges the monoid and identity operators and the braid operator changes to a \((\text{braid})^{-1}\) operator. Noting also that \(x(i\pi - \theta) = x^{-1}(\theta)q^{2(n+1)}\) we obtain:

\[
\check{R}_{1,1}^{(TPG)\text{cross}}(i\pi - \theta) = \frac{x^{-1}q^{2n+2}(1-q^2)}{x^{-1}q^{2n+2} - q^2} \left( \frac{x^{-1}q^{2n+2} - 1}{x^{-1}q^{2n+2} - q^2} \right) \times \\
+ \frac{x^{-1}q^{2n+2}(x^{-1}q^{2n+2} - 1)(1-q^2)}{(x^{-1}q^{2n+2} - q^2)(q^{2n+2} - x^{-1}q^{2n+2})}. \tag{52}
\]

Using relation \((47)\) we can rewrite this in the following form:

\[
\check{R}_{1,1}^{(TPG)\text{cross}}(i\pi - \theta) = \frac{x(1-q^2)(x-q^{2n+2})}{(q^{2n+2} - xq^2)(1-x)} + \frac{q^{2n+2} - x}{q^{2n+1} - xq} \times \\
+ \frac{x(1-q^2)}{q^{2n+2} - xq^2}. \tag{53}
\]

Comparing this with the expression \((51)\) we can see:

\[
\check{R}_{1,1}^{(TPG)\text{cross}}(i\pi - \theta) = \frac{(x-q^2)(x-q^{2n+2})}{(1-x)(q^{2n+2} - xq^2)} \check{R}_{1,1}^{(TPG)}(\theta) . \tag{54}
\]

Writing \(x\) and \(q\) in terms \(\mu\) and \(\omega\) as in \((3)\) we can write the scalar factor

\[
\frac{(x-q^2)(x-q^{2n+2})}{(1-x)(q^{2n+2} - xq^2)} = \frac{\sin(\pi(\mu - \omega))}{\sin(\pi(-\mu + n\omega))} \frac{\sin(\pi(\mu - (n+1)\omega))}{\sin(\pi(-\mu))},
\]

in which the denominator of the factor on the right hand side is equal to its numerator under the transformation \(\theta \to i\pi - \theta\) and therefore we arrive at the desired result:

\[
c_{1,1}(i\pi - \theta)\check{R}_{1,1}^{(TPG)\text{cross}}(i\pi - \theta) = c_{1,1}(\theta)\check{R}_{1,1}^{(TPG)}(\theta), \tag{55}
\]

in which

\[
c_{1,1}(\theta) = \sin(\pi(\mu - \omega))\sin(\pi(\mu - (n+1)\omega)). \tag{56}
\]
C Some formulae concerning \( F_{a,b}(\mu) \)

In this appendix we will derive some important formulae for the scalar factor \( F_{a,b}(\mu) \), introduced in section 3.2, which have been used to calculate the S-matrix elements for the scattering of soliton bound states in section 3.3.

The scalar factor \( F_{1,1}(\mu) \) has been given explicitly in equation (18) in terms of gamma functions. In order to construct breather S-matrices we need the following two identities:

\[
F_{1,1}(\mu + \frac{n+1}{2} \omega) F_{1,1}(\mu - \frac{n+1}{2} \omega) = \frac{\sin(\pi(\mu + \frac{n}{2} \omega - \frac{\omega}{2})) \sin(\pi(\mu - \frac{n}{2} \omega + \frac{\omega}{2}))}{\sin(\pi(\mu - \frac{n}{2} \omega + \frac{\omega}{2})) \sin(\pi(\mu + \frac{n}{2} \omega + \frac{\omega}{2}))} \times \left( \frac{n}{2} \omega + \frac{\omega}{2} \right) \left( \frac{n}{2} \omega + \frac{\omega}{2} + 1 \right) \left( \frac{3}{2} n \omega + \frac{\omega}{2} + 1 \right)
\]

\[
F_{1,1}(\mu + p) = (-1)^p \prod_{l=1}^{p} \frac{[-\omega + l - 1] [\omega + l] [-(n+1)\omega + l - 1] [(n+1)\omega + l]}{[n\omega + l] [(n+2)\omega + l + 1] [l] [l - 1]} F_{1,1}(\mu)
\]

(for any integer \( p \)). (57)

In the last expression we have used the additional notation \([y] \equiv \sin(\frac{\pi}{(n+1)\omega}(\mu + y))\). These formulas can be obtained from (18) by direct calculation\(^{7}\) using the fundamental property of the gamma function \( \Gamma(z+1) = z \Gamma(z) \) (for \( z \neq 0, -1, -2, \ldots \)) and the expansion of sine into an infinite product. (Similar calculations have also been performed in [18].) Together with formula (21) for the general scalar factor \( F_{a,b} \) we can derive the following

\[
F_{a,b}(\mu + \frac{n+1}{2} \omega) F_{a,b}(\mu - \frac{n+1}{2} \omega) = \prod_{j=1}^{a} \prod_{k=1}^{b} \frac{\sin(\pi(\mu + \frac{\omega}{2}(2j + 2k - a - b - 3 + n))) \sin(\pi(\mu + \frac{\omega}{2}(2j + 2k - a - b - 3 + n)))}{\sin(\pi(\mu + \frac{\omega}{2}(2j + 2k - a - b - 1 + n))) \sin(\pi(\mu + \omega(2j + 2k - a - b - 1 + n)))} \times \left( \frac{\omega}{2}(2j + 2k - a - b - 1 + n) \right) \left( \frac{\omega}{2}(2j + 2k - a - b - 1 + n) + 1 \right) \times \left( \frac{\omega}{2}(2j + 2k - a - b - 1 - n) \right) \left( \frac{\omega}{2}(2j + 2k - a - b - 1 + 3n) + 1 \right)
\]

(58)

This last formula reduces to formula (27) in section 3.3 and we see that the infinite product of gamma functions has been reduced to just a finite product of sine functions. From this formula it is relatively straightforward to calculate all S-matrix elements for the scattering of breathers with themselves and of solitons and excited solitons with breathers. The results of these calculations were listed at the end of section 3.3.

\(^{7}\)In all these calculations one has to assume that \( \omega \) is not an integer. This case would correspond to \( q = \text{root of unity which should be examined separately} \).
D Pole structure of rational $c_n$-invariant $S$-matrices

The rational $c_n$-invariant $S$-matrices are given in [26], their $R$-matrix structure being given by the TPG as in section 2, but with $\langle r \rangle$ replaced by $-[r]$ where

$$[r] \equiv \frac{\theta + \frac{i\pi r}{\hbar'}}{\theta - \frac{i\pi r}{\hbar'}},$$

and $U_q(g)$-modules replaced by $g$-modules; and with the ‘minimal’ $S$-matrices ($R$-matrices made crossing symmetric and unitary and without any physical poles) being multiplied by CDD factors equal to the naïve $d_{n+1}^{(2)}$ real ATFT $S$-matrix numerators of [13]. (These would describe Gross-Neveu models. For principal chiral models we would take two copies of the minimal $S$-matrix, acting on the left- and right-global $g$-symmetry modules, and then multiply by a single CDD factor. Thus the pole structure is different [27], although still explained by an analysis similar to that below.) First we should point out that [26] contains a mistake: in the light of (4) we can see that the right-hand side of equation (12) of that paper, describing $S_{a,b}$ ($a \geq b$), should be multiplied by

$$\prod_{i=1}^{b} \prod_{j=1}^{a-1} [a - b + 2i - 2j].$$

For $a + b < n + 1$ the rational $S_{a,b}$ has simple poles at $(a + b)\frac{i\pi}{\hbar'}$, corresponding to the direct-channel fusing $a, b \to a + b$, and at $(b' - a + b)\frac{i\pi}{\hbar'}$, corresponding to the fusing $a, b \to a - b$, and their crossed-channel partners.

There are also double poles at $a - b + 2i$ ($i = 1, \ldots, b - 1$) and $b' + 2j - a - b$ ($j = 1, \ldots, b - 1$). These correspond to diagrams of the form of figure 1,
In figure 6a the direct channel (left-to-right) angle at the internal $S$-matrix is $(a - b)i\pi/h'$, at which it has neither pole nor zero, while in figure 6b the angle is $(h' - a - b)i\pi/h'$, at which $S_{a-j,b-j}$, too, is finite; thus both diagrams give double poles.

For $a + b \geq n + 1$ the situation is different. For $i = 1, \ldots, n - a$ figure 6a still describes a double pole in the same way. In figure 6b, we still have a double pole for $j = 1, \ldots, a + b - n - 2$, but for higher $j$ the internal $S_{a-j,b-j}$ has poles. The correct orders of the poles in $S_{a,b}$, when the zeros arising from the truncation of the TPG have been taken into account (as noted in [25]), are two for $j = a + b - n - 1$, and three for $j = a + b - n, \ldots, b - 1$, and it is these that we must explain. Now the internal $S_{a-j,b-j}$ has poles of order one and two respectively, leading to naive orders for these diagrams of three and four. However, at these internal angles $S_{a-j,b-j}$ projects onto precisely that part of the $(a - j, b - j)$ TPG which is lost in truncation of the $(a, b)$ TPG, giving us an extra zero and the correct pole orders. The only pole we are unable to explain satisfactorily (again as pointed out in [25]) is that at $i\pi/2$ in $S_{a,n+1-a}$, a problem which does not arise either for the principal chiral model $S$-matrix or in the trigonometric case. This mechanism applied to the trigonometric case also gives the correct pole orders for the $p = 0$ poles but fails to explain the higher ones, which we expect to require diagrams of the form of figure 3 or of even higher order.

It is interesting to note that these diagrams plus the tree-level diagrams now explain all the $R$-matrix singularities, at which all the edges directed into a subgraph of the TPG have the same value. Further, we can nest a series of diagrams of the type of figures 6a and 6b, with, say, $i = j = 1$, to give all the singularities of the $R$-matrix in two diagrams, corresponding to the horizontal and vertical links respectively in the TPG. It therefore becomes interesting to consider whether some method along these lines might help us to understand the singularities of other (e.g. $b_n$- or $d_n$-invariant) $R$-matrices whose decomposition is not known. There are intriguing similarities with the singularity theorem of Chari and Pressley [49], who pointed out that the singularity at the crossing point of the $R$-matrix associated with a Lie algebra $\tilde{g}$ must also be a singularity of the $R$-matrix associated with $g$, where the Dynkin diagram of $\tilde{g}$ is a sub-diagram of that of $g$. (Presumably this result also extends to singularities other than that at the crossing point.) This theorem has recently been used powerfully to help understand the fusion properties of $U_q(\tilde{g})$- and Yangian representations [45].

35
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