G\textsuperscript{(1)}\textsubscript{2} Affine Toda Field Theory:  
A Numerical Test of Exact S–Matrix Results

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ABSTRACT

We present the results of a Monte–Carlo simulation of the G\textsuperscript{(1)}\textsubscript{2} Affine Toda field theory action in two dimensions. We measured the ratio of the masses of the two fundamental particles as a function of the coupling constant. Our results strongly support the conjectured duality with the D\textsuperscript{(3)}\textsubscript{4} theory, and are consistent with the mass formula of Delius et al.

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1 Introduction

An affine Toda field theory is a theory of scalar fields in two dimensions with exponential interactions. There is an affine Toda field theory associated with each Kac–Moody algebra, with the interactions given by the simple roots of the algebra. If we denote the fields by \( \phi^i \), and the simple roots of the Kac–Moody algebra by \( \alpha^i_a \), then the action takes the form

\[
S = \int d^2x \left\{ \frac{1}{2} \partial^\mu \phi \cdot \partial_\mu \phi + \frac{m^2}{\beta^2} \sum_a n_a \exp(\beta \alpha \cdot \phi) \right\},
\]

(1)

where \( \beta \) is the coupling constant, \( m \) is the mass scale and \( n_a \) are numbers chosen so that \( \phi = 0 \) is the minimum of the potential. What makes the Toda theories special is that classically they are integrable with conserved quantities whose spins are given by the exponents of the affine algebra. The presence of higher spin conserved quantities in the quantum theory implies that the scattering preserves individual particle momenta, and that the S–matrix factorises on the two particle scatterings. For details of Kac–Moody algebras and their classification see e.g. [1]. Each algebra is denoted \( G_n^{(r)} \) where \( G_n \) is a finite dimensional Lie algebra and \( r \) is the twist, which can be 1, 2 or 3. \( G_n^{(r)} \) has \( n+1 \) simple roots which span \( \mathbb{R}^n \). To each simple root \( \alpha \) of a Kac–Moody algebra we can associate a dual root, \( \alpha^\vee \), given by \( \alpha^\vee = 2\alpha/|\alpha|^2 \). These dual roots are also the simple roots of a Kac–Moody algebra. If the algebra and its dual are isomorphic, then we call that algebra (Langlands) self–dual. The self dual algebras are \( A_{1}^{(1)}, D_{2}^{(1)}, E_{6}^{(1)}, A_{2}^{(2)} \), and the non-self dual algebras come in dual pairs \( (B_{n}^{(1)} , A_{2n-1}^{(2)} ), (C_{n}^{(1)}, D_{2n-2}^{(2)} ), (G_{2}^{(1)}, D_{4}^{(3)} ), (F_{4}^{(1)}, E_{6}^{(2)}) \).

Although all the divergences can be removed from a two dimensional scalar theory by normal ordering, at first sight the action (1) appears to present difficulties in that there will be an infinite set of counterterms generated and that these will not necessarily preserve the form of the action which depends on only two constants \( m, \beta \). However, it can be shown that normal ordering only induces a multiplicative change in the exponentials. Thus, for any theory of \( n \) fields with \( n+1 \) exponential interactions all regulation schemes are equivalent up to a constant shift in the scalar fields and a renormalisation of \( m \), provided that any \( n \) of the \( n+1 \) directions \( \alpha_a \) are linearly independent [2, 3]. The Affine Toda theories are therefore renormalisable and it makes sense to discuss the \( \beta \)–dependence of physical observables since this coupling constant is unaltered by a change in the regulation scheme.

Since the mass scale \( m \) depends on the regulation scheme, it is only the ratios which are observable. It is a remarkable fact that to first order in perturbation theory the mass ratios for the self–dual theories are independent of the coupling constant and keep their classical values [4, 5]. This feature enables one to write down simple S–matrices which have their physical poles fixed at the fusion angles given by the classical masses and allowed tree-level three point couplings. The S-matrix coupling dependence is then added in so as to agree with first order perturbation theory [4–6]. However this procedure does not work for the non-self dual theories. There are two reasons. Firstly, the bootstrap constraint on the S–matrices does not close on the classical particles; and secondly, the mass ratios are renormalised by quantum effects even in first order perturbation theory. However, by performing a careful analysis of the first order perturbation theory and requiring that the two particle S–matrices obey certain relations (crossing-symmetric, unitarity and a bootstrap hypothesis), Delius et al. were able to postulate the S–matrices of these theories.
One of the new features of these S-matrices as compared to the self-dual theories is that the position of the poles is now $\beta$ dependent. These S-matrices thus provide predictions for the mass ratios of the Toda theories in the large $\beta$, non-perturbative regime. The mass ratios which they found exhibit a relation between the dual theories: the mass ratios in one theory for large coupling constant are the same as those in the dual theory for small coupling constant. Furthermore the S–matrices for two dual theories may both be expressed as the same function when written in terms of a parameter $B$ which encodes the coupling constant behaviour, and the only difference between the two theories is the dependence of this function $B$ on the coupling constant. Further evidence for this duality can be found by looking for the quantum conserved currents [9–11], which also exhibit this property; the conserved currents for small $\beta$ for one theory have the same form as the conserved currents for large $\beta$ of the dual theory [11].

In this paper we present the results of a Monte-Carlo simulation of the $G^{(1)}_2$ Affine Toda field theory. The convention used for the $G^{(1)}_2$ roots was,

$$\alpha_1 = (\sqrt{2}, 0), \quad \alpha_2 = (-1/\sqrt{2}, -\sqrt{3}/2), \quad \alpha_3 = (-1/\sqrt{2}, 1/\sqrt{6}).$$  

The corresponding constants $n_a$ are $n_1 = 2, n_2 = 1, n_3 = 3$. The S–matrix prediction of Delius at al. [8, 12] for the ratio of the masses of two fundamental particles of this theory is

$$\frac{m_2}{m_1} = \frac{\sin(2\pi/H)}{\sin(\pi/H)},$$

where

$$H = 6 + (\beta^2/2\pi)/(1 + (\beta^2/12\pi)).$$

This agrees with perturbation theory to one loop. The $G^{(1)}_2$ theory is dual to the $D^{(3)}_4$ theory ($H$ flows from 6 to 12 with increasing $\beta$ – the twist times the Coxeter numbers of $G^{(1)}_2$ and $D^{(3)}_4$ respectively). The prediction is that for small $\beta$ the mass ratio for the $G^{(1)}_2$ theory is approximately $\sqrt{3}$, and for large $\beta$ it approaches the classical value of the $D^{(3)}_4$ theory, which is $\sqrt{(\sqrt{3} + 1)/(\sqrt{3} - 1)}$. We have measured the flow of the mass ratios as a function of $\beta$. Our observations strongly support the duality conjecture and are consistent with the functional form of this flow (3).

The rest of the letter is laid out as follows. In sect. 2 we present the simulation details, and in sect. 3 we summarise our results and compare them with prediction. Finally we present our conclusions.

### 2 Simulation Details

A Metropolis simulation was carried out on a periodic square lattice (most runs using a $64 \times 40$ lattice). The discrete Euclidean action used was

$$S = \frac{1}{2} \sum_{nm} (\phi_n - \phi_m) \cdot (\phi_n - \phi_m) + \frac{m^2}{\beta^2} \sum_{n, a} n_a \exp(\beta \alpha_a \cdot \phi_n),$$

where $n$ labels a site and the first sum is over nearest-neighbour sites. Measurements of the zero spatial momentum components of the three correlation functions $\langle \phi^1(x, t)\phi^1(0, 0) \rangle$,
\[ \langle \phi^1(x,t)\phi^2(0,0) \rangle, \langle \phi^2(x,t)\phi^2(0,0) \rangle \] and of the two field averages \( \langle \phi^1(0) \rangle \) and \( \langle \phi^2(0) \rangle \) were made. Labelling the sites by their spatial and time coordinates the correlation functions were calculated in the following way (the short lattice direction is characterised as the spatial direction and the long length as the time direction):

\[
\langle \phi^i(n_t)\phi^j(0) \rangle = \frac{1}{L} \sum_{m=1}^{L} \left( \frac{1}{N} \sum_{n=1}^{N} \phi^i_{n,m} \right) \left( \frac{1}{N} \sum_{n'=1}^{N} \phi^j_{n',m+n_t} \right)
\]

where \( N \) and \( L \) are the lattice lengths in the spatial and time directions respectively. The matrix of correlation functions was fitted by the function

\[
\begin{pmatrix}
\langle \phi^1(n_t)\phi^1(0) \rangle & \langle \phi^1(n_t)\phi^2(0) \rangle \\
\langle \phi^1(n_t)\phi^2(0) \rangle & \langle \phi^2(n_t)\phi^2(0) \rangle \\
\end{pmatrix} =
\begin{pmatrix}
S_1 & S_1 & S_1 & S_2 \\
S_2 & S_1 & S_2 & S_2 \\
\end{pmatrix}
\]

\[+ R(\theta_1) \begin{pmatrix} ae^{-m_1 n_t} & 0 \\ 0 & 0 \end{pmatrix} R^{-1}(\theta_1) + R(\theta_2) \begin{pmatrix} 0 & 0 \\ 0 & be^{-m_2 n_t} \end{pmatrix} R^{-1}(\theta_2),
\]

where \( R(\theta) \) is the rotation matrix

\[
R(\theta) = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}
\]

\( m_1 \) and \( m_2 \) the two masses, \( a \) and \( b \) constants, and \( S_1 \) and \( S_2 \) correspond to the vacuum expectation values of the fields. Since we imposed periodic boundary conditions on our lattice, we should be fitting to a more complicated function that \( (7) \), with exponentials replaced by coshes. In each case, the fitted parameters were insensitive to this because the statistical errors in the correlation functions grew with separation.

On fitting to various separations we found that the differences between the fitted values of \( \theta_1, \theta_2 \) were of the order of the statistical errors (~1%). We then chose to fit the correlation functions with \( (7) \) on separations for which the effective masses (derived assuming \( \theta_1 = \theta_2 \)) were approximately constant. In practice this meant that fits to \( (7) \) were carried out over separations \( n_t \) from 0 out to some larger distance which varied between 4 and 15.

The eight parameter fit of \( (7) \) was carried out with a standard chi-squared minimisation routine. The chi-squared function involved a sum over contributions from the three correlation functions at each of the separations being fitted plus the two field averages. The errors in the denominator of the chi-squared function were obtained by rebinning the data in order to allow for computer time autocorrelations (this rebinning method involves averaging the data into successively fewer bins until the variance of a particular parameter over the bins converges [13]). A bootstrap routine was carried out over the binned data in order to obtain the error estimates on the fitted parameters. If there were \( N_{bin} \) bins of data, then the bootstrap method involved choosing \( N_{bin} \) new bins randomly from these bins (with repetition when it occurred), fitting our function over this new data set, and then repeating over an ensemble of such data sets. The variances of the fitted parameters over this ensemble gave the quoted errors.

The simulation was carried out by choosing a particular \( \beta \) value, and then decreasing \( m \) in \( (5) \) until the measured mass ratio converged to within statistical errors (this is the scaling requirement that must be met in order that a lattice theory can give information about the continuum). Finite-size effects were then examined for those values of \( \beta \) for which scaling was observed by varying the spatial lattice size.
3 Results

The results are collected in figures 1 and 2a – 2f. 10000 equilibration iterations and 809200 further iterations were carried out to obtain each mass ratio measurement. Each such run on the $64 \times 40$ lattice required approximately 120 hours of CPU time on a Sparc IPC machine. Figure (1), shows measurements of the mass ratio at two different masses in equation (1), at a selection of $\beta$ values on the $64 \times 40$ lattice. The solid line is the prediction (4) of Delius et al [8]. Figures 2a – 2f show all runs for each of the $\beta$ values. These latter plots show the masses plotted against the longer of the two correlation lengths measured. In addition, the $\beta = 50$ and $\beta = 20$ plots (figures 2a and 2b) show the results of runs carried out on $64 \times 60$ and $64 \times 30$ lattices.

In order that scaling is achieved, the points on figures 2a – 2f must reach a plateau as the correlation length increases. The absence of finite-size effects must then be demonstrated for points that lie on this plateau.

All the points for $\beta = 50$ and $\beta = 20$ on the $64 \times 40$ lattice vary by less than one percent and lie well within each other’s (one sigma) error bars. Furthermore, the results on the lattices with smaller and larger spatial dimensions agree to the same accuracy. Thus these two criteria are taken as having been met.

For the other $\beta$ values, the situation is less clear cut. As $\beta$ was decreased it became necessary to go to larger correlation length to achieve finite size scaling and the error bars increased in size due to critical slowing down. Nevertheless for $\beta = 5$ and $\beta = 2$ scaling seems to have been achieved. However finite-size effects may be important at these longer correlation lengths (finite-size effects were examined in detail for correlation lengths of approximately 1.5 at $\beta = 20$ and 50, compared to the correlation lengths of 3-4 relevant here). For $\beta = 1$ and $\beta = 0.01$, the perturbative regime, scaling has not been adequately established (to do this would require larger lattices and longer runs).

On figure 1 we show a selection of points from the simulations on a $64 \times 40$ lattice as follows: the shortest two correlation length points from each of figures 2a and 2b - which lie on the plateaus and have smaller error bars than the longer correlation length points; the 3 longer correlation points from figure 2c - scaling has not been reached for the shortest correlation length point; all the points from figures 2d to 2f - for which scaling has not been adequately established.

From figure 1, the $\beta = 20$ and $\beta = 50$ data strongly support the duality conjecture (that the mass ratio flows to the 1.93 value shown corresponding to the mass ratio for $D_{4}^{(3)}$) in the $\beta \to 0$ limit. As discussed above this is the data for which systematic errors associated with scaling and finite-size effects are most under control. The rest of the data is consistent with the prediction of Delius et al. over the complete $\beta$ value range.

4 Conclusions

It is clear that our results are in agreement with the predictions of duality; that is that the large $\beta$ limit of the mass ratio in the $G_{2}^{(1)}$ affine Toda is the same as small $\beta$ limit of the mass ratio in the $D_{4}^{(3)}$ theory. In addition our results for the intermediate $\beta$ range are not significantly different from the ratio predicted by Delius et al. [8].

Monte-Carlo simulations might also provide a non-perturbative check on other theoretical predictions. For example there is some dispute as to the meaning of the anomalous
threshold singularities in the $S$–matrices of Delius et al. A careful calculation of the one-loop corrections and of the conservation of the charges by Delius et al. showed that some of the poles which one would like to assign to fundamental particles are displaced by loop effects. It is not clear whether this signals new particles or not. It should in principle be able to test whether these do indeed correspond to physical states by measuring higher-order correlation functions. In addition it should prove possible to check the proposed form factor formulae from similar measurements. Perhaps more immediately, one can investigate whether the observed duality is present in the $D_{4}^{(3)}$ theory, and in the other non self-dual rank two Affine Toda theories. We hope to be able to report on these questions in the future.

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6 References

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## Table of collected data

| $\beta$ | $L$   | $m$ | $m_2/m_1$ | $\delta(m_2/m_1)$ | $m_1$  | $m_2$  |
|---------|-------|-----|-----------|-------------------|--------|--------|
| 50      | $64 \times 60$ | $10^{-9}$ | 1.9208 | 0.0073 | 0.7584 | 1.4568 |
|         | $64 \times 40$  | $10^{-9}$ | 1.9302 | 0.0082 | 0.7599 | 1.4669 |
|         | $64 \times 30$  | $10^{-9}$ | 1.9271 | 0.0077 | 0.7563 | 1.4575 |
|         | $64 \times 40$  | $10^{-10}$ | 1.9317 | 0.0074 | 0.6705 | 1.2952 |
|         | $64 \times 40$  | $10^{-13}$ | 1.9344 | 0.0017 | 0.3629 | 0.7019 |
|         | $64 \times 40$  | $10^{-20}$ | 1.9456 | 0.0155 | 0.3227 | 0.6279 |
| 20      | $64 \times 60$ | $10^{-4}$  | 1.9235 | 0.0193 | 0.5873 | 1.1296 |
|         | $64 \times 40$  | $10^{-4}$  | 1.9292 | 0.0108 | 0.5847 | 0.1128 |
|         | $64 \times 30$  | $10^{-4}$  | 1.9234 | 0.0146 | 0.5846 | 1.1244 |
|         | $64 \times 40$  | $10^{-5}$  | 1.9330 | 0.0108 | 0.4334 | 0.8377 |
|         | $64 \times 40$  | $10^{-6}$  | 1.9216 | 0.0175 | 0.3217 | 0.8637 |
|         | $64 \times 40$  | $10^{-7}$  | 1.9276 | 0.0224 | 0.2393 | 0.4613 |
| 5       | $64 \times 40$  | $0.1$     | 1.8524 | 0.0119 | 0.5156 | 0.8437 |
|         | $64 \times 40$  | $0.07$    | 1.8821 | 0.0116 | 0.4294 | 0.8082 |
|         | $64 \times 40$  | $0.05$    | 1.8832 | 0.0155 | 0.3685 | 0.6940 |
|         | $64 \times 40$  | $0.03$    | 1.8921 | 0.0180 | 0.2891 | 0.5471 |
| 2       | $64 \times 40$  | $0.1$     | 1.8089 | 0.03   | 0.2203 | 0.3986 |
|         | $64 \times 40$  | $0.14$    | 1.8029 | 0.0172 | 0.2872 | 0.5179 |
| 1       | $64 \times 40$  | $0.35$    | 1.7083 | 0.03   | 0.5255 | 0.8975 |
|         | $64 \times 40$  | $0.3$     | 1.7151 | 0.0105 | 0.4560 | 0.7822 |
|         | $64 \times 40$  | $0.18$    | 1.7365 | 0.0148 | 0.2828 | 0.4911 |
|         | $64 \times 40$  | $0.14$    | 1.7424 | 0.0294 | 0.2268 | 0.3952 |
|         | $64 \times 40$  | $0.12$    | 1.7832 | 0.0235 | 0.1889 | 0.3369 |
| 0.01    | $64 \times 40$  | $0.4$     | 1.6898 | 0.017  | 0.5598 | 0.9459 |
|         | $64 \times 40$  | $0.25$    | 1.7035 | 0.02   | 0.3564 | 0.6071 |
|         | $64 \times 40$  | $0.2$     | 1.7302 | 0.0260 | 0.2826 | 0.4889 |
|         | $64 \times 40$  | $0.15$    | 1.7061 | 0.0257 | 0.2149 | 0.3667 |