Monte Carlo study of exact S-matrix duality
in non simply laced affine Toda theories

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(June 22, 2021)

**Abstract**

The \((g_2^{(1)}, d_4^{(3)})\) pair of non simply laced affine Toda theories is studied from the point of view of non perturbative duality. The classical spectrum of each member is composed of two massive scalar particles. The exact S-matrix prediction for the dual behaviour of the coupling dependent mass ratio is found to be in strong agreement with Monte Carlo data.

keywords: Affine Toda theories, exact S-matrix, bootstrap principle.

PACS numbers: 11.10.Lm, 02.20.Fh, 11.10.Gh, 11.10.Kk
I. INTRODUCTION

Affine Toda field theories are two-dimensional models described by the Euclidean action

$$S = \int d^2 x \left( \frac{1}{2} \partial_\mu \phi \cdot \partial_\mu \phi + \frac{m^2}{\beta^2} \sum_{a=0}^{r} n_a e^{\beta \alpha^{(a)} \cdot \phi} \right).$$

(1.1)

The $r$-dimensional vectors $\{\alpha^{(a)}\}$ are the simple roots of an affine Kac-Moody algebra [1] and $\{n_a\}$ are positive integers depending on the algebra and satisfying

$$\sum_a n_a \alpha_a = 0, \quad n_0 = 1.$$  

(1.2)

The field $\phi$ is a set of $r$ real scalar components. Finally, $m$ and $\beta$ are a mass scale parameter and the coupling constant. The Coxeter number is the positive integer $h = n_0 + \cdots + n_r$.

Under the transformation $T : \alpha \to 2\alpha/|\alpha|^2$, the lattice of the simple roots transforms into the lattice of another affine algebra. The invariant algebras are called self-dual; they belong to the untwisted a-d-e series $a_n^{(1)}$, $d_n^{(1)}$, $e_n^{(1)}$ and to the twisted series $a_{2n}^{(2)}$. The other algebras are the pairs $(b_n^{(1)}, a_{2n-1}^{(2)})$, $(c_n^{(1)}, d_{2n-1}^{(2)})$, $(g_2^{(1)}, d_4^{(3)})$, and $(f_4^{(1)}, e_6^{(2)})$; they are invariant under $T$.

At the classical level, affine Toda theories have no coupling; $\beta$ can be scaled away, the spectrum is proportional to $m$, independent of $\beta$ and moreover it is given by simple universal formulae in terms of the Coxeter number. The interest of the classical theory is that the field equations of motion admit a Lax pair and therefore there is an infinite hierarchy of conserved currents with increasing spin.

At the quantum level, this property is inherited in the form of a factorized S-matrix. The dependence on $\beta$ which plays the role of Planck’s constant becomes non trivial; on the other hand the parameter $m$ becomes unphysical due to renormalization effects and only mass ratios are observables.

Since the S-matrix is expected to be factorizable, its explicit form may be sought. One can make a guess and impose physical constraints like unitarity or crossing symmetry and the additional bootstrap principle. In the case of the self-dual theories, perturbation theory
suggests that the mass ratios do not renormalize. Indeed, the bootstrap equations close on an ansatz for the S-matrix based on the tree level spectrum and on the fusings allowed by the three-point couplings [2,3].

Perturbation theory and the structure of the bootstrap suggest conjectured expressions for the exact $\beta$ dependence of the S-matrix which show a remarkable duality between weak and strong coupling in terms of the transformation $\beta \rightarrow 4\pi/\beta$.

As pointed out in [4], for the non self dual pairs the picture is more complicated. Mass ratios deform already at the lowest order of perturbation theory and the simplest ansatz for the S-matrix fails.

However, a non trivial solution to the bootstrap equations can be found with the feature of predicting $\beta$ dependent mass ratios [5,6]. The predictions are then formally the same as in the classical theory, but in terms of a “renormalized” Coxeter number $H(\beta)$.

Again, the explicit non perturbative form of $H(\beta)$ is not known. The simplest conjecture [10], consistent with low order perturbation theory [9] and current algebra [7] predicts a new kind of duality. Under $\beta \rightarrow 4\pi/\beta$ the S-matrices of the pair members get exchanged. Hence, the strong coupling regime in one theory should be given by the weak coupling regime in the other.

In [8] a Monte Carlo study of duality in the pair $(g_{2}^{(1)}, d_{4}^{(3)})$ was performed by mean of the Metropolis algorithm. The authors determined the mass ratio in the $g_{2}^{(1)}$ theory over a wide range of couplings and they did find agreement with the duality conjecture. Specifically, they checked that the mass ratio in $g_{2}^{(1)}$ ranged between its classical values and the classical value of $d_{4}^{(3)}$.

In this paper I carried over the above simulation on larger lattices with higher statistics in order to pin down the precise dependence on $\beta$. Moreover, I have used the Hybrid Monte Carlo algorithm [13]. Finally, I have extended the simulation to the $d_{4}^{(3)}$ theory in order to have a complete picture.

The plan of the paper is the following: Section II describes the pair $(g_{2}^{(1)}, d_{4}^{(3)})$; Section III shows the one loop deformations of the mass ratios; Section IV gives some detail on the
II. THE DUAL PAIR \( (G_2^{(1)}, D_4^{(3)}) \)

The pair \( (g_2^{(1)}, d_4^{(3)}) \) has \( r = 2 \) and its action is

\[
S = \int d^2x \left\{ \frac{1}{2} \partial_{\mu} \phi \cdot \partial_{\mu} \phi + \frac{m^2}{\beta^2} \sum_{a=0}^{n_a} \exp(\beta \alpha_a \cdot \phi) \right\}, \quad \phi = (\phi_1, \phi_2). \tag{2.1}
\]

The integers \( n_a \) and the simple roots are

\[
g_2^{(1)}: n = \{2, 3, 1\}, \quad \alpha = \left\{ \left( \sqrt{2}, 0 \right), \left( -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{6}} \right), \left( -\frac{1}{\sqrt{2}}, -\frac{\sqrt{3}}{2} \right) \right\}; \tag{2.2}
\]

\[
d_4^{(3)}: n = \{2, 1, 1\}, \quad \alpha = \left\{ \left( \sqrt{2}, 0 \right), \left( -\frac{3}{\sqrt{2}}, \frac{\sqrt{3}}{2} \right), \left( -\frac{1}{\sqrt{2}}, -\frac{\sqrt{3}}{2} \right) \right\}. \tag{2.3}
\]

The two sets of roots are related by the duality \( \alpha \to 2\alpha/|\alpha|^2 \).

The two corresponding models are very different at the tree level. The explicit expansion of the mass-potential exponential term up to the fourth order for the \( g_2^{(1)} \) model is

\[
V(\phi_1, \phi_2) = m^2 \left( 3 \phi_1^2 + \phi_2^2 \right) + 
+ m^2 \beta \frac{9 \phi_1^3 - 9 \phi_1 \phi_2^2 - 2 \sqrt{3} \phi_2^3}{9 \sqrt{2}} + 
+ m^2 \beta^2 \frac{27 \phi_1^4 + 18 \phi_1^2 \phi_2^2 + 8 \sqrt{3} \phi_1 \phi_2^3 + 7 \phi_2^4}{72} + O(\beta^3). \tag{2.4}
\]

For the \( d_4^{(3)} \) model we utilize the tree level mass eigenstates by transforming the fields

\[
\phi \to R\phi, \quad R = \begin{pmatrix}
\cos \theta & \sin \theta \\
-\sin \theta & \cos \theta
\end{pmatrix}, \quad \theta = \frac{5\pi}{12} \tag{2.5}
\]

and obtain the expansion

\[
V(\phi_1, \phi_2) = m^2 \left( (3 - \sqrt{3}) \phi_1^2 + (3 + \sqrt{3}) \phi_2^2 \right) + 
+ m^2 \beta \left( \frac{\phi_1^3}{2} - \frac{\sqrt{3} \phi_1^3}{2} + \frac{3 \phi_1^2 \phi_2}{2} - \frac{\sqrt{3} \phi_1^2 \phi_2}{2} + \frac{3 \phi_1 \phi_2^2}{2} + \frac{\sqrt{3} \phi_1 \phi_2^2}{2} + \frac{\phi_2^3}{2} + \frac{\sqrt{3} \phi_2^3}{2} \right) + 
+ m^2 \beta^2 \left( 7 \phi_1^4 - \frac{5 \phi_1^4}{4 \sqrt{3}} + \frac{\phi_1^4 \phi_2}{2} - \frac{\phi_1^4 \phi_2}{2} + \frac{3 \phi_1^2 \phi_2^2}{4} + \frac{\phi_1^2 \phi_2^2}{2} + \frac{\phi_1 \phi_2^3}{\sqrt{3}} + \frac{\phi_1 \phi_2^3}{\sqrt{3}} + \frac{7 \phi_2^4}{8} + \frac{5 \phi_2^4}{4 \sqrt{3}} \right) + O(\beta^3) \tag{2.6}
\]
As one can see, the sets of possible fusings are completely different and duality is far from being obvious. The classical mass ratios are

\[
\frac{m_2}{m_1}_{g_2^{(1)}} = \sqrt{3}, \quad \frac{m_2}{m_1}_{d_4^{(3)}} = \sqrt{\frac{\sqrt{3} + 1}{\sqrt{3} - 1}} = \sqrt{2} \quad (2.7)
\]

which agree with the general formula in terms of the Coxeter number \( h \) (6 for \( g_2^{(1)} \), 12 for \( d_4^{(3)} \))

\[
\frac{m_2}{m_1} = \frac{\sin(2\pi/h)}{\sin(\pi/h)} = 2 \cos(\pi/h) \quad (2.8)
\]

The duality conjecture states that the correct quantum ratio \( g_2^{(1)} \) is given by substituting \( h \to H(\beta) \) in the model \( g_2^{(1)} \) and \( h \to H(4\pi/\beta) \) in the \( d_4^{(3)} \) model. The form of \( H(\beta) \) is constrained but not fixed by perturbation theory and the conjectured expression is

\[
H(\beta) = 6 + \frac{\beta^2/2\pi}{1 + \beta^2/12\pi} \quad (2.9)
\]

Let us clarify these statements by considering the one loop mass ratios.

**III. ONE LOOP MASS RATIOS**

Let us denote the three diagrams of Figures (I-II-III) by

\[
\Gamma_{abc}^{(1)}, \quad \Gamma_{abcd}^{(2)}, \quad \Gamma_{abcd}^{(3)} \quad (3.1)
\]

where \( a, b, c \) and \( d \) are particle labels in the range \( \{1, 2\} \). The mass ratio is observable since renormalization amounts to a normal ordering of the exponentials and its effect is a redefinition of the bare mass. We must check that in a bare renormalization scheme all the divergent tadpole graphs cancel. Let us utilize dimensional regularization and let us introduce

\[
Z_i = \int \frac{d^dp}{(2\pi)^d} \frac{1}{p^2 + m_i^2} \quad (3.2)
\]

The pole part of \( Z_i \) is mass independent, hence the cancellation is a matter of couplings. At the one loop level the mixed propagator corrections are irrelevant and we can restrict to the diagonal ones. Let us write the interaction lagrangian in the form
\[ V(\phi_1, \phi_2) = \frac{1}{2} (m_1^2 \phi_1^2 + m_2^2 \phi_2^2) + V_{111} \phi_1^3 + V_{112} \phi_1^2 \phi_2 + \cdots. \] (3.3)

Then, the corrections to the propagator of particle 1 are

\[ \Gamma_{111}^{(1)} = -12 V_{111} Z_1, \]
\[ \Gamma_{112}^{(1)} = -2 V_{112} Z_2, \]
\[ \Gamma_{1111}^{(2)} = 18 V_{111}^2 Z_1 m_1^{-2}, \]
\[ \Gamma_{1112}^{(2)} = 6 V_{111} V_{112} Z_2 m_1^{-2}, \]
\[ \Gamma_{1121}^{(2)} = 2 V_{112}^2 Z_1 m_2^{-2}, \]
\[ \Gamma_{1122}^{(2)} = 6 V_{112} V_{222} Z_2 m_2^{-2}. \] (3.4)

The corrections to the propagator of particle 2 are obtained by exchanging the 1 and 2 labels. If we denote the full divergent correction by

\[ \delta m_1^2 = \Gamma_{111}^{(1)} + \Gamma_{112}^{(1)} + \Gamma_{1111}^{(2)} + \Gamma_{1112}^{(2)} + \Gamma_{1121}^{(2)} + \Gamma_{1122}^{(2)}, \] (3.5)

then the desired cancellation is equivalent to the condition

\[ \frac{\delta m_1^2}{m_1^2} = \frac{\delta m_2^2}{m_2^2}. \] (3.6)

which is indeed satisfied by the couplings of the two theories which can be read in the expansions of the previous section.

Besides the consistency check, let us turn to the mass ratio deformation. At one loop, we must determine the quantity

\[ \delta \frac{m_1^2}{m_2^2} = \frac{m_1^2}{m_2^2} \left( \frac{\delta m_1^2}{m_1^2} - \frac{\delta m_2^2}{m_2^2} \right). \] (3.7)

Let us introduce the finite integral

\[ Z_{ij}(p^2) = \int \frac{d^2 q}{(2\pi)^2} \frac{1}{(q^2 + m_i^2)((q + p)^2 + m_j^2)}, \] (3.8)

Then the finite contributions to the propagators of particle 1 are
\[ \Gamma_{1111}^{(3)} = 18V_{111}^2 Z_{11}(p^2), \]
\[ \Gamma_{1112}^{(3)} = 4V_{112}^2 Z_{12}(p^2), \]
\[ \Gamma_{1122}^{(3)} = 2V_{122}^2 Z_{22}(p^2). \]

(3.9)

Evaluation on the tree mass shell gives

\[- \delta m_1^2 = 18V_{111}^2 Z_{11}(-m_1^2) + 4V_{112}^2 Z_{12}(-m_1^2) + 2V_{122}^2 Z_{22}(-m_1^2) \]

(3.10)

with analogous expressions for the particle 2. We need only the following particular values

\[ Z_{ii}(-m_i^2) = \frac{1}{4\sqrt{3}m_i^2}; \]
\[ Z_{ij}(-m_i^2) = \frac{1}{2\pi \sqrt{m_j^2(m_j^2 - 4m_i^2)}} \text{ArcTanh} \sqrt{\frac{m_j^2 - 4m_i^2}{m_j^2}} \]

(3.11)

(3.12)

and the final result is

\[ g_2^{(1)}: \quad \delta \frac{m_2^2}{m_2^2} = \frac{1}{12\sqrt{3}} \beta^2 + O(\beta^4); \quad d_4^{(3)}: \quad \delta \frac{m_4^2}{m_4^2} = -\frac{1}{16} \beta^2 + O(\beta^4). \]

(3.13)

The renormalized Coxeter number is thus

\[ g_2^{(1)}: \quad H(\beta) = 6 + \frac{\beta^2}{2\pi} + O(\beta^4); \quad d_4^{(3)}: \quad H(\beta) = 12 - \frac{9\beta^2}{2\pi} + O(\beta^4) \]

(3.14)

and a consistent, simple and natural conjecture is

\[ g_2^{(1)}: \quad H(\beta) = H_0(\beta); \quad d_4^{(3)}: \quad H(\beta) = H_0(4\pi/\beta) \]

(3.15)

where

\[ H_0(\beta) = 6 + \frac{\beta^2/2\pi}{1 + \beta^2/12\pi} \quad 6 < H_0 < 12. \]

(3.16)

The result for \( g_2^{(1)} \) is in agreement with that quoted by [3]. The result for \( d_4^{(3)} \) gives perturbative support to the duality conjecture \( \beta \to 4\pi/\beta \). We remark that the discrepancy with [3] is due to the fact that they use the form of \( H_0 \) which is correct for the simply laced models.
IV. DETAILS OF THE SIMULATION

The lattice action for the pair \((g_2^{(1)}, d_3^{(3)})\) expressed in terms of pure numbers is

\[
S_{\text{Toda}} = \sum_{n \in \text{sites}} \left\{ \frac{1}{2} \sum_{\mu=1,2} (\phi_{n+\mu} - \phi_n)^2 + \frac{m^2}{\beta^2} \sum_{a=1}^3 n_a \exp(\beta \alpha_a \cdot \phi) \right\}, \quad \phi = (\phi_1, \phi_2). \tag{4.1}
\]

I have simulated the Toda theory with the Hybrid Monte Carlo algorithm (see [13] for the details). Let us consider the extended action

\[
S = S_p + S_{\text{Toda}}, \tag{4.2}
\]

\[
S_p = \frac{1}{2} \sum_n \pi_n \cdot \pi_n, \quad \pi = (\pi_1, \pi_2). \tag{4.3}
\]

The free parameter of the algorithm are \(N_{\text{hmc}}\) and \(\epsilon\). The first is the number of molecular dynamics steps. The second is the time step in the integration of the equations of motion

\[
\dot{\phi}_n = \pi_n, \tag{4.4}
\]

\[
\dot{\pi}_n = \sum_\mu (\phi_{n+\mu} - 2\phi_n + \phi_{n-\mu}) - \frac{m^2}{\beta} \sum_a n_a \alpha_a \exp(\beta \alpha_a \cdot \phi_n). \tag{4.5}
\]

The vacuum expectation value of the field is a non physical quantity. However, it is interesting to measure it since it is an indicator of thermalization and also because it is in a sense a dynamic minimum of the Toda potential.

Mass ratios can be determined by studying the eigenvalues of the two point function

\[
\langle 0| \Phi_i(0) \Phi_j(\tau) |0 \rangle - \langle 0| \Phi_i |0 \rangle \langle 0| \Phi_j |0 \rangle \tag{4.6}
\]

where \(t\) is the lattice time ranging from 0 to \(T\) and the wall field \(\Phi_i(t)\) is obtained by averaging \(\phi\) over space.

V. RESULTS

I have used a \(80^2\) lattice for all \(\beta\)s because the correlation lenght may be adjusted by varying \(m\). The continuum mass ratio is independent of the bare mass \(m\). However, on a finite lattice, it must be chosen in order to have correlation lenghts large with respect to one
lattice spacing and small compared to the lattice size. This is the correct procedure which minimizes discretization and finite size corrections. Thanks to the work of [8] I had good values in the case of the $g_{2}^{(1)}$ theory. In the other model, I started with the same values of $m$ adjusting them for some $\beta$.

I utilized different measurement of the wall-wall two-point function for each bin in the separation $\tau$. This is necessary in order to avoid strong correlation between data.

Table I shows the Hybrid Monte Carlo parameters which we found to be optimal for each couple $(\beta, m)$. The time step $\epsilon$ must be reduced almost exponentially as $\beta$ is increased. This is reasonable since at larger $\beta$ the potential profile becomes steeper.

Table II shows the measure of $\langle 0|\phi_{i}|0 \rangle$ which can be useful as a check of the code and which is needed in order to subtract the two-point function.

Table III shows the two lattice masses, their ratio and the conjectured prediction.

Finally, tables IV, V, VI show the same results in the case of the $d_{4}^{(3)}$ model.

Figures I-II-III show the self energy diagrams which are needed in order to compute the one loop mass ratio deformations.

Figure IV shows a summary plot of the measured mass ratios in the two models together with the conjectured ones and the asymptotic values holding in the classical limit.

VI. CONCLUSIONS

In this paper I have investigated numerically the conjectured duality in the pair $(g_{2}^{(1)}, d_{4}^{(3)})$ of non simply laced affine Toda theories. I have shown that the $\beta$ dependence of the mass ratios in $g_{2}^{(1)}$ does follows the behaviour conjectured in [8] and that the data of $d_{4}^{(3)}$ agree with the $\beta \to 4\pi/\beta$ duality.

As in the case of more realistic field theories like QCD, the numerical approach could be useful in studying other interesting features of quantum Toda theories. For instance, one could try to find direct evidence of the boundary bound states which appears when the theory is restricted to a half-line [11]; work is in progress on this topic. Moreover, it could be
valuable a non perturbative study of the solitons which appear at imaginary \( \beta \), and which suggests that a unitary theory can ultimately be found by restricting the state space of the hamiltonian \([12]\); their stability is indeed still questionable \([14]\).

VII. ACKNOWLEDGEMENTS

I gratefully acknowledge G. M. T. Watts and R. A. Weston for useful suggestions and interest.
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CAPTIONS

Fig. I-II-III : self energy one loop diagrams.

Fig. IV : summary of the numerical results.
TABLES

TABLE I. $g_2^{(1)}$: HMC parameters.

| $\beta$ | $N_{hmc}$ | $\epsilon$ |
|---------|-----------|------------|
| 1.0     | 10        | 0.1        |
| 2.0     | 10        | 0.08       |
| 3.5     | 10        | 0.07       |
| 5.0     | 10        | 0.06       |
| 10.0    | 5         | 0.05       |
| 20.0    | 10        | 0.025      |

TABLE II. $g_2^{(1)}$ bare mass and dynamical minimum.

| $\beta$ | $m$     | $\langle \phi_1 \rangle$  | $\langle \phi_2 \rangle$ |
|---------|---------|-----------------------------|-----------------------------|
| 1.0     | 0.1     | -0.0982(6)                  | 0.225(1)                    |
| 2.0     | 0.1     | -0.1542(4)                  | 0.3768(8)                   |
| 3.5     | 0.05    | -0.2073(5)                  | 0.5300(9)                   |
| 5.0     | 0.01    | -0.2752(4)                  | 0.6866(8)                   |
| 10.0    | 5E-5    | -0.3396(7)                  | 0.843(1)                    |
| 20.0    | 5E-7    | -0.2362(4)                  | 0.7023(7)                   |
### TABLE III. \( g_2^{(1)} \): mass ratio.

| \( \beta \) | \( m_1 \)       | \( m_2 \)       | \( R \)   | \( R^* \)  |
|------------|----------------|----------------|----------|------------|
| 1.0        | 0.1595(2)      | 0.27839(5)     | 1.745(2) | 1.74509    |
| 2.0        | 0.2133(2)      | 0.3784(1)      | 1.775(2) | 1.77605    |
| 3.5        | 0.2262(5)      | 0.41192(5)     | 1.821(5) | 1.82579    |
| 5.0        | 0.1615(4)      | 0.3004(1)      | 1.861(5) | 1.86150    |
| 10.0       | 0.1379(3)      | 0.2630(2)      | 1.908(5) | 1.90870    |
| 20.0       | 0.2896(3)      | 0.5576(1)      | 1.926(3) | 1.92562    |

### TABLE IV. \( d_4^{(3)} \): HMC parameters.

| \( \beta \) | \( N_{\text{hmc}} \) | \( \epsilon \) |
|------------|---------------------|--------------|
| 1.0        | 10                  | 0.07         |
| 2.0        | 10                  | 0.08         |
| 3.5        | 10                  | 0.05         |
| 3.5        | 10                  | 0.06         |
| 5.0        | 10                  | 0.05         |
| 10.0       | 10                  | 0.02         |
| 10.0       | 10                  | 0.03         |
| 20.0       | 10                  | 0.0125       |
TABLE V. $d_4^{(3)}$ bare mass and dynamical minimum.

| $\beta$ | $m$ | $\langle \phi_1 \rangle$ | $\langle \phi_2 \rangle$ |
|---------|-----|-----------------|-----------------|
| 1.0     | 0.1 | 0.1530(5)       | -0.1930(9)      |
| 2.0     | 0.1 | 0.2014(3)       | -0.2210(6)      |
| 3.5     | 0.05| 0.2305(2)       | -0.2174(4)      |
| 3.5     | 0.01| 0.3163(5)       | -0.3687(9)      |
| 5.0     | 0.01| 0.2701(3)       | -0.2552(5)      |
| 10.0    | 5E-5| 0.3061(3)       | -0.2729(6)      |
| 10.0    | 1E-7| 0.4410(8)       | -0.504(1)       |
| 20.0    | 5E-7| 0.2488(2)       | -0.1489(4)      |

TABLE VI. $d_4^{(3)}$: mass ratio.

| $\beta$ | $m_1$  | $m_2$  | $R$    | $R^*$  |
|---------|--------|--------|--------|--------|
| 1.0     | 0.2166(1)| 0.4149(1) | 1.916(2) | 1.91665 |
| 2.0     | 0.3363(2)| 0.6323(1) | 1.880(1) | 1.88120 |
| 3.5     | 0.3427(1)| 0.6280(1) | 1.832(1) | 1.82840 |
| 3.5     | 0.2150(1)| 0.3931(3) | 1.829(1) | 1.82840 |
| 5.0     | 0.3850(2)| 0.6903(4) | 1.793(2) | 1.79398 |
| 10.0    | 0.3506(6)| 0.6155(3) | 1.756(4) | 1.75193 |
| 10.0    | 0.1201(3)| 0.2106(1) | 1.753(6) | 1.75193 |
| 20.0    | 0.5727(6)| 0.9966(6) | 1.740(2) | 1.73740 |
