NUMERICAL STUDY OF THE MASS SPECTRUM IN THE 2D O(3) $\sigma$ MODEL WITH A THETA TERM

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INTRODUCTION

It has been recently conjectured [1,2] that the spectrum of the \( O(3) \) non–linear \( \sigma \) model in 2 dimensions with a theta term contains a singlet and a triplet states. Their masses (called \( m_S \) and \( m_T \) respectively) would depend on \( \theta \) as shown in the sketch:

![Fig. 1](image)

The triplet mass is represented by the continuous line and the singlet mass by the dashed line. Notice that as \( \theta \to 0 \) the triplet mass tends to the value \( m_{HMN} \) which is the exact mass gap calculated in Ref. [3] (and numerically verified with a 2–3% precision in Ref. [4]). At \( \theta = \pi \) the states become massless [5] (see Refs. [6,7] for a Monte Carlo analysis).

The values of the masses at the extremes of the interval \( \theta \in [0, \pi] \) induce the conjecture that there exists an intermediate critical \( \theta_c \) where the singlet mass \( m_S \) becomes twice the triplet mass \( m_T \). We present a progress report on a project where all these features about the spectrum of the model are numerically analyzed.
We have regularized the 2–dimensional O(3) $\sigma$ model on the lattice by using the standard action

\[ S_L = A_L - i\theta_L Q_L , \]
\[ A_L \equiv -\beta \sum_{x,\mu} \vec{\phi}(x) \cdot \vec{\phi}(x + \hat{\mu}) , \]
\[ Q_L \equiv \sum_x Q_L(x) , \]  

(1)

where $\vec{\phi}(x)$ is a 3–component unit vector that represents the dynamical field variable, $\beta$ is the inverse bare lattice coupling constant for this standard regularization and $\theta_L$ is the bare theta parameter. The lattice operator for the density of topological charge is defined as in Ref. [8]

\[ Q_L(x) = \frac{1}{32\pi} \epsilon^{\mu\nu} \epsilon_{abc} \phi^a(x)(\phi^b(x+\hat{\mu})-\phi^b(x-\hat{\mu}))(\phi^c(x+\hat{\nu})-\phi^c(x-\hat{\nu})) . \]  

(2)

The use of the above topological charge density entails an inconvenience and a benefit. The former is that the total topological charge on a single configuration $Q_L$ in general does not take on integer numbers. The benefit is that with this expression one can write down an efficient cluster algorithm to hasten the simulation runs (see below).
THE TOPOLOGICAL CHARGE ON THE LATTICE

In a general regularization, the bare topological charge density operator renormalizes through the expression

$$ Q_L = Z_Q Q, \quad (3) $$

where $Q$ is the continuum definition of the operator. For the 2–dimensional O(3) sigma model the topological charge operator has no anomalous dimensions and thus $Z_Q$ is always free of cutoff divergences. This renormalization constant depends only on the coupling constant.

Values of operators on single configurations do not make sense in Field Theory since the relevant quantities in the Theory are the expectation values of the operator. On the lattice they are calculated as an average over many configurations. The formal mathematical expression (3) means that any expectation value that contains $n$ insertions of $Q$ and which is calculated by the regularization $Q_L$ requires a factor of $(Z_Q)^n$ (contact terms are not relevant for the purposes of the present work).

In the study of the spectrum of the O(3) sigma model with a $\theta$ term, the renormalization constant $Z_Q$ is required in two places:

- $i$) The end point of the masses lies at $\theta_{\text{end}} = \pi$ (see Figure 1). Then the following expression holds: $\pi = Z_Q \theta_{L,\text{end}}$ where $\theta_{L,\text{end}}$ is the value of the end point determined from our simulations. We can calculate $Z_Q$ independently (see next page) and verify that the results match.

- $ii$) The critical point where $m_S$ becomes twice the triplet mass $m_T$ renormalizes in the same fashion: $\theta_c = Z_Q \theta_{L,c}$. We can check our calculations by verifying that the same $\theta_c$ is extracted from different values of $\beta$ (recall that $Z_Q$ is a function of the coupling constant).
CALCULATION OF $Z_Q$

An independent value of the renormalization constant $Z_Q$ can be obtained by using the so–called heating method [9].

Since $Z_Q$ renormalizes the operator $Q$ (see Eq.(3)), then one may obtain its estimate by applying a few updating (heating) steps on a classical topological charge 1 instanton placed by hand on the lattice. To monitor the background topological charge, a cooling procedure is applied on the configuration after each updating step. When the background topological charge is changed (it is no longer 1) the heating procedure is stopped. The value of $\langle Q_L\rangle$ before stopping usually displays a plateau. This plateau is the value of $Z_Q$.

The figure shows an example of the procedure. The value of $\langle Q_L\rangle$ begins at 1 and it decreases as the updating goes ahead. The plateau is manifest.

Fig. 2
The sign problem that afflicts the model described by the action in Eq. (1) precludes a direct Monte Carlo simulation. Therefore we have simulated the model for imaginary values of theta, $\theta_L = -i \theta_L$, and the results will be extrapolated to the real $\theta$.

The model described by the action in Eq. (1–2) with an imaginary $\theta$ can be simulated by using a cluster algorithm [10, 11].

The first part at each updating step in the Wolff algorithm for the standard O(3) sigma model without a theta term consists in choosing a random unit vector $\vec{r}$ in such a way that every dynamical field can be split in a component parallel to $\vec{r}$ and the rest, $\vec{\phi}(x) = \left( \vec{\phi}(x) \cdot \vec{r} \right) \vec{r} + \vec{\phi}_\perp(x)$, where $\vec{\phi}_\perp(x)$ denotes the part of $\vec{\phi}(x)$ orthogonal to $\vec{r}$. Then the signs of $\left( \vec{\phi}(x) \cdot \vec{r} \right)$ for all $x$ are updated à la Swendsen–Wang as in the Ising model.

Now apply the same separation in components parallel and perpendicular to $\vec{r}$ to the theory with a theta term. With this separation the lattice density of topological charge $Q_L(x)$ can be rewritten as

$$Q_L(x) = \frac{1}{16\pi} \left\{ \left( \vec{\phi}(x) \cdot \vec{r} \right) (d_{1,2} + d_{-1,-2} + d_{2,-1} + d_{-2,1}) + \right.$$

$$\left( \vec{\phi}(x + \hat{1}) \cdot \vec{r} \right) (d_{0,-2} - d_{0,2}) + \left( \vec{\phi}(x - \hat{1}) \cdot \vec{r} \right) (d_{0,2} - d_{0,-2}) +$$

$$\left( \vec{\phi}(x + \hat{2}) \cdot \vec{r} \right) (d_{0,1} - d_{0,-1}) + \left( \vec{\phi}(x - \hat{2}) \cdot \vec{r} \right) (d_{0,-1} - d_{0,1}) \right\},$$

where $x \pm \hat{1}$ means the site at the position one step forward (backward) in the direction “1” starting from site $x$ (we have only two directions, “1” and “2”) and the notation $d_{i,j}$ stands for the $3 \times 3$ determinant.
IMAGINARY $\theta$ (II)

(the three components for each vector are unfold along the rows)

$$d_{i,j} \equiv \det \begin{pmatrix} \vec{r} & \vec{\phi}(x + \hat{i}) \\ \vec{\phi}(x + \hat{j}) \end{pmatrix}. \quad (4)$$

In this fashion the theory, with an imaginary theta, at each updating step looks like an Ising model in the presence of an external local magnetic field $h(x)$ because the $\theta$-term has become linear in the dynamical field $\vec{\phi}$. One can readily derive that the magnetic field at site $x$ is

$$h(x) = \frac{\partial L}{16\pi} |\vec{\phi}(x) \cdot \vec{r}| \left( d_{1,2} + d_{-1,-2} + d_{2,-1} + d_{-2,1} + d_{-1,-1,-2} + \\
ed_{-1+2,-1} + d_{1,1+2} + d_{1-2,1} + d_{2,2-1} + d_{2+1,2} + \\
ed_{-2,-2+1} + d_{-2-1,-2} \right). \quad (5)$$

d_{i+k,j}$, and analogous terms in (5), are the straightforward generalization of the above definition (4) when the site is obtained by shifting two steps ($\hat{i}$ plus $\hat{k}$) from the original position $x$.

Thus we have converted the original theory in an Ising model in the presence of a local external magnetic field (which changes at each updating step and therefore it must be recalculated at each step). In the literature there are two cluster algorithms expressly introduced to update Ising models in the bosom of magnetic fields: the Lauwers–Rittenberg [12] and the Wang [13] methods. We have chosen the latter since it is more adequate for the use of improved estimators [14] when extracting correlation functions.
OBSERVABLES

At $\theta \neq 0$ physical states are not characterized by their parity, but only by their $O(3)$ group contents. Therefore we have used two interpolating operators of either parity for both states in order to allow the model to choose the correct parity mixture. The two pairs of operators are

$$O^1_T \equiv \vec{\phi}(x), \quad O^2_T \equiv -i\vec{\phi}(x) \times \vec{\phi}(x + \hat{1}),$$

(6)

for the triplet and

$$O^1_S \equiv \vec{\phi}(x) \cdot \vec{\phi}(x + \hat{1}), \quad O^2_S \equiv -i\vec{\phi}(x) \cdot \left(\vec{\phi}(x + \hat{1}) \times \vec{\phi}(x - \hat{1})\right),$$

(7)

for the singlet. Then the corresponding wall operators have been built by averaging over the $x_1$ coordinate ($L$ is the lattice size)

$$W^i_T \equiv \frac{1}{L} \sum_{x_1} O^i_T, \quad W^i_S \equiv \frac{1}{L} \sum_{x_1} O^i_S, \quad i = 1, 2,$$

(8)

and their correlation functions evaluated by a numerical simulation.

Let us fix our attention on the triplet state (the same remarks will apply also to the singlet case). In order to extract the correct parity mixture for the physical particle and to clean the signal from possible excited states, we adopted the variational method of Refs. [15,16]:

- i) compute the connected cross–correlation matrix among the wall operators,

$$C^{ij}_T(x_2) = \langle W^i_T(x_2)W^j_T(0) \rangle - \langle W^i_T(0) \rangle \langle W^j_T(0) \rangle,$$

(9)

- ii) diagonalize $C^{ij}_T(x_2)$ for each $x_2$ obtaining the eigenvalues $\lambda^\alpha_T(x_2)$ (it can be easily checked that all eigenvalues are real) and finally

- iii) extract a set of masses $m^\alpha_T$ by fitting the function

$$\lambda^\alpha_T(x_2) = c_0 + c_1 \cosh \left( a m^\alpha_T \left( \frac{L}{2} - x_2 \right) \right),$$

(10)

where $a$ is the lattice spacing. The lowest among all results is the sought singlet mass, $am_T = \min_{\alpha} \{am^\alpha_T\}$. 
NUMERICAL RESULTS (I)

We have simulated the model at several values of $\vartheta$ on a lattice at $\beta = 1.5$ and 1.6. The lattice size was $L = 120$ in the first case and $L = 180$ in the second case. These sizes allow a loose ratio of $L$ over the correlation length $L/\xi$ which guarantees the absence of relevant finite size effects. We have alternated hits of the above cluster algorithm with over–heat–bath steps [17] and measured $2 \cdot 10^5$ propagators on as many independent configurations for all values of $\vartheta$ and $\beta$.

We show the results regarding the triplet mass and its cut on the $\theta^2$ axis. They are displayed in Figure 3 with the extrapolation from imaginary $\theta$ ($\theta^2 < 0$) to real $\theta$ for $\beta = 1.5$ and 1.6. The data points lie in the negative $\theta^2$ sector. The extrapolation has been performed by using several functional forms. In Figure 3 we show the extrapolation which
yielded the best statistical test $\chi^2/(\text{d.o.f.})$. It was a ratio of two 4th degree polynomials and the above test was 1.1 for $\beta = 1.5$ and 0.4 for $\beta = 1.6$.

From the fits we can obtain the values of $Z_Q(\beta)$ for the two $\beta$ at which the study was performed. By imposing $\pi = Z_Q\theta_L$, end we obtain:

<table>
<thead>
<tr>
<th>Table 1</th>
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<td>$(\theta_{L,\text{end}}(\beta = 1.5))^2$</td>
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<tr>
<td>$Z_Q(\beta = 1.5)$</td>
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<tr>
<td>$(\theta_{L,\text{end}}(\beta = 1.6))^2$</td>
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<td>$Z_Q(\beta = 1.6)$</td>
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The $Z_Q$ from the heating method are displayed in the following Table:

<table>
<thead>
<tr>
<th>Table 2</th>
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<tbody>
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<td>$Z_Q(\beta = 1.5)$</td>
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<tr>
<td>$Z_Q(\beta = 1.6)$</td>
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they are in excellent agreement with the values obtained from the spectrum analysis. Let us explain several details of the heating calculation of $Z_Q$. 
NUMERICAL RESULTS (III)

We ran $10^4$ trajectories of 100 Heat–Bath steps each for the two values of $\beta$. In the Figure we show the average plateau for the case of $\beta = 1.5$.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig4.png}
\caption{\label{fig:4} $\beta=1.5$}
\end{figure}

The initial instanton was
\begin{equation}
\frac{\phi^1 + i\phi^3}{1 - \phi^2} = \frac{z - z_c}{\rho e^{i\pi/4}},
\end{equation}
where $z \equiv x_1 + ix_2$, $z_c$ is its center location and $\rho$ is the size. The size was chosen in such a way that the inequalities $\rho < 0.15La$ and $\rho > 8a$ hold [18,19]. The value of the plateau was normalized to the topological charge of the initial instanton, Eq.(11). Six cooling steps were performed after every heating step and the trajectory was rejected from the step where the background charge was found not equal to 1 (within a tolerance $\delta = 0.2$) [20]. In this fashion we possibly rejected a few trajectories that contained the correct instanton background ($Q = 1$) but at least we are completely sure that no wrong backgrounds ($Q \neq 1$) were included in the analysis to obtain the values of $Z_Q(\beta)$ in Table 2.
CONCLUSIONS

• We have numerically simulated the 2–dimensional non–linear O(3) \( \sigma \) model with a \( \theta \) term in order to study its spectrum as \( \theta \) varies. In Figure 1 we show the expected behaviour of the spectrum. This expectation was obtained by analyzing the model as a deformation of the integrable theory at \( \theta = \pi \) [1,2,5].

• The usual standard action on the lattice was used as a Boltzmann weight. This choice brings about large systematic errors in the computation of masses (see for example Ref. [4]). However, we are interested only in ratios of masses and the location where they vanish and both these issues are not affected by such errors.

• To apply usual importance sampling we have made a Monte Carlo simulation of the theory at imaginary \( \theta \). Then the results are extrapolated to real \( \theta \).

• We have introduced a modification of the Wolff algorithm for the usual O(3) model in order to efficiently simulate the theory at imaginary \( \theta \). The new algorithm is fast and allows the use of improved estimators for (few fields) correlation functions.

• In Figure 3 we show the results of the extrapolation for the triplet mass at two different values of the coupling constant. The point where the extrapolated curves cut the \( \theta^2 \) axis is equal to \( (\pi/Z_Q(\beta))^2 \). Thus our results allow to extract the renormalization constant \( Z_Q \) for different \( \beta \) (see Table 1). This constant can then be compared with the extraction from more usual techniques like the so–called “heating method” [9]. The agreement is excellent (see Table 2).

• We have obtained a topology property of the model by studying its mass spectrum.
REFERENCES


