Proceedings of the International School-seminar
"New Physics and Quantum Chromodynamics at External Conditions", pp. 90 – 93,
May 22-24, 2013, Dnipropetrovsk, Ukraine

$2D$ $O(3)$ SIGMA MODEL WITH θ-TERM: CONSTRUCTION OF A POSITIVE BOLTZMANN WEIGHT

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The continuum limit of the dual formulation of the two-dimensional lattice $SU(N)$ principal chiral model is constructed. The continuum action is in general complex and appears to be a functional of an $(N^2 - 1)$-component non-compact scalar field. As an application of this construction we establish a relation between the dual of the $SU(2)$ principal chiral model and the $O(3)$ non-linear sigma model with a θ-term in the continuum limit. This relation is exact when the radial part of the scalar dual field is taken to be a constant. Therefore, the dual formulation of the lattice $SU(2)$ model with constant radial part can be regarded as a non-perturbative regularization of the $O(3)$ model with θ term. Furthermore, under certain conditions one could construct a positive definite dual Boltzmann weight. This property enables us to prospect Monte Carlo simulations of $O(3)$ with a θ term at *real* values of θ.

1 Introduction

In this paper we discuss the continuum limit of the dual formulation of the two-dimensional ($2D$) $SU(N)$ principal chiral model. Our chief interest relies on the fact that upon certain condition on the dual field, the resultant model for $N = 2$ turns out to be a valid discretization of the $2D$ $O(3)$ non-linear sigma model with a θ term.

While at $\theta = 0$ the $O(3)$ model is integrable [1] with a spectrum exhibiting a massive triplet of scalars [2,3], the physics of this model gets notoriously enriched when the topological parameter θ is switched on. At $\theta = \pi$ it has been argued that the theory is massless (Haldane conjecture) [4–10]. Then, as θ gets lower starting from $\theta = \pi$, the spectrum develops a massive singlet along with the previously mentioned triplet with masses $m_S(\theta)$ and $m_T(\theta)$ respectively. In particular these masses are proportional to $(\pi - \theta)^{\frac{2}{3}}$ for values of θ that are close to π from below [11]. It has been shown, [12–15], that $m_S(\theta)$ is permanently larger than $m_T(\theta)$. Since at $\theta = 0$ the spectrum is exclusively composed by the triplet, it has been conjectured that at some critical value $0 < \theta_c < \pi$ the mass $m_S(\theta_c)$ becomes exactly twice $m_T(\theta_c)$ in such a way that for any $\theta < \theta_c$ the singlet copiously decays into states belonging to the triplet. Finally, as $\theta \to 0$ the value of $m_S(\theta)$ should diverge, thus leaving the theory without θ bereft of the singlet state.

Monte Carlo simulations on the lattice are a unique tool to probe the physical properties of any statistical model. For the case at hand, numerical computer simulations could greatly help in clarifying the particle content and the θ-dependence of their masses. However, a straightforward attempt to simulate the model by discretizing its action is doomed to failure because the topological θ-term is pure imaginary. Only at $\theta = 0$ the problem completely disappears. This is a heavy drawback as importance sampling, which lies at the root of the Monte Carlo process, applies only as long as Boltzmann weights are strictly positive. Thus, one could only simulate the model at imaginary values of θ when the Boltzmann weight becomes positive. In [16] the Haldane conjecture has been verified by extrapolating the mass derived at imaginary values of θ towards the real θ-axis.

The $2D$ $O(3)$ non-linear sigma model with a non-zero θ term is not the only theory afflicted by the above problem. Also QCD at finite quark density cannot be directly simulated because the chemical potential is pure imaginary. None of the known methods provides information about the singlet state and the θ dependence of its mass. Therefore, new simulation algorithms able to examine the model well within the region of real finite θ would be very welcome. In this contribution we derive a non-perturbative regularization for the $2D$ $O(3)$ non-linear sigma model with θ term. This regularization enables us to construct a positive Boltzmann weight which, thus, can be used for Monte Carlo simulations of the model.

We shall work on a $2D$ lattice $\Lambda \in Z^2$ with lattice spacing a and a linear extension L. Periodic boundary conditions are imposed in both directions. Let us define three partition functions:

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1. Partition function of the lattice $SU(N)$ principal chiral model in the link formulation [17–19]

$$Z_{SU(N)} \;=\; \int \prod_l dV(l) \exp\left[\beta \sum_l \mathrm{Tr}V(l)\right] \prod_x \left[\sum_r d(r)\chi_r(V_x)\right] \;, \tag{1}$$

   where $V(l)$ is the $SU(N)$ matrix associated to the link l, $d(r)$ is the dimension of the representation r and $\chi_r(V_x)$ is the character of the r-th representation. The matrix V_x is defined as

$$V_x \;=\; V(l_1)V(l_2)V^{\dagger}(l_3)V^{\dagger}(l_4) \;=\; \exp[i\lambda_k\ \omega_k(x)] \;. \tag{2}$$

   Here, l_i are 4 links attached to the site x. The expression $\sum_r d(r)\chi_r(V_x)$ is the $SU(N)$ delta-function which introduces the constraint $V_x = 1$ on the link matrices (local Bianchi identity).

2. We shall use also the following partition function

$$Z(\beta, R) \;=\; \int \prod_l dV(l) \exp\left[\beta \sum_l \mathrm{Tr}V(l)\right] \prod_x \frac{\sin R\ \omega(x)}{\sin \omega(x)} \;. \tag{3}$$

   Here, $\omega(x) = (\sum_{k=1}^{3} \omega_k^2(x))^{\frac{1}{2}}$ and $\omega_k(x)$ are the angles parameterizing the $SU(2)$ matrix in (2). R is an arbitrary real number. If $R = 2r + 1$ with r taking integer and half-integer values then the expression under the product over x in the last formula is an $SU(2)$ character and the partition function (3) can be regarded as being obtained from (1) by fixing all representations to some constant. Since delta-function is not present, we refer to the model (3) as unconstrained $SU(2)$ model.

3. The partition function of the $O(3)$ non-linear sigma model with a θ-term in the continuum is given by

$$Z_{O(3)} \;=\; \int \prod_{k=1}^{3} D\sigma_k(x)\ \exp\left[-\frac{1}{2}\beta_{O(3)} \int d^2x(\partial_\mu \sigma_k(x))^2 + i\theta S_q\right] \;. \tag{4}$$

   The integration is performed with the constraint $\sum_{k=1}^{3} \sigma_k^2(x) = 1$. The θ-term or topological action S_q reads

$$S_q \;=\; \int \frac{d^2x}{8\pi}\ \epsilon^{\mu\nu}\epsilon^{knm}(\partial_\mu\sigma_k)(\partial_\nu\sigma_n)\sigma_m \;. \tag{5}$$

Below we address the following problems:

- construction of the continuum limit of the $SU(N)$ principal chiral model in the link formulation (1);
- as an application of this construction we establish an exact relation between the $O(3)$ non-linear sigma model with a θ-term and the continuum limit of the unconstrained $SU(2)$ model;
- derivation of a positive definite Boltzmann weight.

2 Continuum limit of the $SU(N)$ principal chiral model

The construction of the continuum limit of the $SU(N)$ principal chiral model (1) uses essentially one basic fact: when $\beta \to \infty$ all link matrices perform only small fluctuations around the unit matrix (for a thorough discussion of this property, see [18]; for a rigorous proof, see [20]). More precisely, any configuration of the link matrix for which $\omega_k(l) > \mathcal{O}(1/\sqrt{\beta})$ is exponentially suppressed and becomes singular in the continuum limit. On smooth configurations the Bianchi constraint $V_x = 1$ can only be satisfied when $\omega_k(x) = 0$ for all $k = 1, \ldots, N^2 - 1$. Therefore, the $SU(N)$ delta-function can be replaced by the Dirac delta-functions

$$\sum_r d(r)\chi_r(V_x) \;\longrightarrow\; \prod_{k=1}^{N^2-1} \int_{-\infty}^{\infty} e^{i\alpha_k(x)\omega_k(x)}\ d\alpha_k(x) \;. \tag{6}$$

Then, the continuum limit for smooth configurations can be constructed in the standard way:

1. introduce dimensionful vector potentials $\omega_k(l) = aA_k(l)$ and expand the action and angles $\omega_k(x)$ in powers of the lattice spacing a;
2. replace the $SU(N)$ invariant measure by a flat measure and extend the integration region over potentials $A_k(l)$ to the non-compact region $A_k(l) \in [-\infty, \infty]$;
3. in the limit $a \to 0$ finite differences are replaced by derivatives and sums by integrals.

Neglecting terms which vanish in the limit $a \to 0$ one gets a Gaussian integral over vector fields $A_k(l)$. Integration over $A_k(l)$ produces a local continuum theory for the dual scalar potentials $\alpha_k(x)$ which can be written as

$$Z_{SU(N)} \;=\; \int_{-\infty}^{\infty} e^{-S_{\mathrm{eff}}} \prod_{k=1}^{N^2-1} d\alpha_k(x) \; . \tag{7}$$

The effective continuum action reads

$$S_{\mathrm{eff}} \;=\; \frac{1}{4}\int d^2x \;\left(\partial_\mu \alpha_k(x)\right)\; M^{kn}_{\mu\nu}\;\left(\partial_\nu \alpha_n(x)\right) - \frac{1}{2}\int d^2x \;\; \ln \mathrm{Det} M \; , \tag{8}$$

where the inverse of the matrix M is given by

$$\left[M^{kn}_{\mu\nu}\right]^{-1} \;=\; \beta\, \delta_{\mu\nu}\, \delta_{kn} \;-\; i\epsilon^{\mu\nu}\, f^{knm}\, \alpha_m(x) \; . \tag{9}$$

Here we turn our attention to the specific model with $N = 2$. In this case $f^{knm} = \epsilon^{knm}$ and both $\mathrm{Det}M$ and the matrix M can be easily deduced. Let us make the change of variables $\alpha_k(x) = R(x)\,\sigma_k(x)$, $\sum_{k=1}^{3}\sigma_k^2(x) = 1$. By substituting the last formulas into (7) we get for the continuum limit of the $SU(2)$ principal chiral model

$$Z_{SU(2)} = \int_0^{\infty} \prod_x \frac{R^2(x)dR(x)}{\beta\,(\beta^2 + R^2(x))} \int \prod_x \left[\delta(1 - \sum_{k=1}^{3}\sigma_k^2(x)) \prod_{k=1}^{3} d\sigma_k(x)\right] \exp\left[- \int d^2x\; \mathcal{L}(R(x), \sigma_k(x))\right] , \tag{10}$$

$$\mathcal{L}(R(x), \sigma_k(x)) \;\equiv\; \frac{1}{4}\;\left(\partial_\mu[R(x)\sigma_k(x)]\right)\; M^{kn}_{\mu\nu}\;\left(\partial_\nu[R(x)\sigma_n(x)]\right) \; , \tag{11}$$

$$M^{kn}_{\mu\nu} \;=\; \frac{1}{\beta^2 + R^2(x)}\;\left[\delta_{\mu\nu}\left(\beta\delta_{kn} + \frac{R^2(x)}{\beta}\sigma_k(x)\sigma_n(x)\right) + iR(x)\;\epsilon^{\mu\nu}\;\epsilon^{knm}\;\alpha_m(x)\right] \; . \tag{12}$$

Consider the $SU(2)$ model obtained above on a constant configuration $R(x) = R = \mathrm{const}$. Noting that $\sum_k \sigma_k(x)\partial_\mu\sigma_k(x) = 0$, one can see that the Lagrangian (11) becomes that of the $O(3)$ sigma model with a θ term. Moreover, this constant radial part R of the dual field $\alpha_k(x)$ can be identified with the parameter R introduced in the unconstrained $SU(2)$ model (3). Indeed, up to terms of order $\mathcal{O}(a^4)$ which vanish in the continuum limit, the factor $\sin R\omega/\sin\omega$ in (3) can be represented as

$$\frac{\sin R\omega}{\sin\omega} \;\approx\; R\frac{\sin R\omega}{R\omega} \;=\; R \int \delta\left(1 - \sum_{k=1}^{3}\sigma_k^2\right)\prod_{k=1}^{3} d\sigma_k\; e^{iR\omega_k\sigma_k} \; . \tag{13}$$

Using the above calculations for the $SU(2)$ principal chiral model and formula (13) we can easily compute the continuum limit of the unconstrained $SU(2)$ model obtaining the following relation between partition functions

$$Z_{O(3)} \;=\; \left[C(\beta, R)\right]^{L^2}\; Z(\beta, R) \; , \tag{14}$$

valid in the continuum limit. The relation between the couplings in both models can be read off from the Lagrangian (11) by taking $R(x) = R$ and comparing it with the Lagrangian of the $O(3)$ model. We have for the direct relation

$$\beta_{O(3)} = \frac{\beta}{2}\,\frac{R^2}{R^2 + \beta^2} \; , \; \theta = 2\pi R\,\frac{R^2}{R^2 + \beta^2} \; . \tag{15}$$

3 Positive Boltzmann weight

As is seen from (14), the unconstrained $SU(2)$ model does provide a lattice non-perturbative regularization for the $O(3)$ model with real θ. Its Boltzmann weight is real but not necessarily positive. Here we re-write the model in a form such that the Boltzmann weight becomes positive definite. To do that let us consider the following expansion into $SU(2)$ characters

$$\frac{\sin R\omega}{\sin\omega} \;=\; \sum_r A_r(R)\;\chi_r(\omega) \; , \tag{16}$$

where the sum runs over all non-negative integers and half-integers and the coefficients $A_r(R)$ of the expansion are given by

$$A_r(R) \;=\; \{\,\delta_{r,s}\; , \text{ if } R = 2s + 1, s = 0, 1/2, 1, ... \frac{2\sin\pi R}{\pi}\;\frac{(-1)^{(2r+1)}(2r + 1)}{R^2 - (2r + 1)^2}, \text{ otherwise} \; . \tag{17}$$

Then, the partition function (3) appears as

$$Z(\beta,R) \;=\; \sum_{\{r(x)\}} \prod_x \; A_{r(x)}(R)\; \tilde{Z}(\beta,R;[r(x)]) \;, \tag{18}$$

$$\tilde{Z}(\beta,R;[r(x)]) \;=\; \int \prod_l dV(l) \exp\left[\beta \sum_l \mathrm{Tr}V(l)\right] \prod_x \; \chi_{r(x)}(V_x) \;. \tag{19}$$

Note that if R were integer then $Z(\beta,R)=\tilde{Z}(\beta,R;[r(x)])$.

Expressing V_x as a product of link matrices (2) the $SU(2)$ characters turn out to be a sum over magnetic numbers. This yields the partition function

$$\tilde{Z}(\beta,R;[r(x)]) \;=\; \prod_x \left[\sum_{\{m_i(x)=-r(x)\}}^{r(x)}\right] \prod_l Q_0(l) \;, \tag{20}$$

$$Q_0(l) \;=\; \int dV e^{\beta \mathrm{Tr}V} \; V_{r(x)}^{m_i(x)\;\, m_{i+1}(x)} \; V_{r(x+e_n)}^{\dagger\; m_j(x+e_n)\;\, m_{j+1}(x+e_n)} \;, \tag{21}$$

where $V_r^{m\;m'}$ indicates the m,m' matrix element of an $SU(2)$ matrix in representation r. There are 4 magnetic numbers $m_i(x)$ $(i=1,2,3,4)$ per lattice site x. The result of the invariant integration can be expanded into a Clebsch-Gordan (CG) series as (up to a sign factor which cancels after multiplication over links)

$$Q_0(l) \;=\; \sum_{J,k} \frac{C_J(\beta)}{2J+1} C^{J\;\,k}_{r(x)\;\, m_i(x)\;\, r(x+e_n)\;\, -m_{j+1}(x+e_n)}\; C^{J\;\,k}_{r(x)\;\, m_{i+1}(x)\;\, r(x+e_n)\;\, -m_j(x+e_n)} \;, \tag{22}$$

with coefficients $C_J(\beta)$ given by

$$C_J(\beta) \;=\; \frac{2J+1}{\beta} I_{2J+1}(2\beta) \;, \tag{23}$$

where $I_{2J+1}(2\beta)$ is the modified Bessel function of first kind. Formulas (18), (20) and (22) define our representation for the partition function of the unconstrained $SU(2)$ model. The new Boltzmann weight, $Q_0(l)$, appears to be always positive on all allowed configurations of the magnetic numbers $m_i(x)$ and representations $r(x)$.

4 Summary

In this paper we have calculated the continuum limit of the dual representation of the $2D$ $SU(N)$ principal chiral model. As an application we have derived a new lattice regularization for the $O(3)$ non-linear sigma model with the θ term. The major advantage of our regularization is that it can be written in a form with strictly positive Boltzmann weight. This opens a possibility for numerical simulations of the model at real values of θ and, therefore for attacking the problems listed in the Introduction from first principles. The work in this direction is now in progress.

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