Testing the heating method with perturbation theory

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Abstract

The renormalization constants present in the lattice evaluation of the topological susceptibility can be non-perturbatively calculated by using the so-called heating method. We test this method for the $O(3)$ non-linear $\sigma$-model in two dimensions. We work in a regime where perturbative calculations are exact and useful to check the values obtained from the heating method. The result of the test is positive and it clarifies some features concerning the method. Our procedure also allows a rather accurate determination of the first perturbative coefficients.

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I. INTRODUCTION

Matrix elements of local operators can be determined by lattice techniques. The corresponding Monte Carlo simulation provides the continuum value of the matrix element modified by lattice finite renormalizations. The renormalization constants are usually evaluated perturbatively. They can also be evaluated by using non-perturbative methods. These methods yield the renormalization constants at any value of the bare coupling $g_0$ avoiding the uncertainties derived from the knowledge of only the few first terms in the perturbative series and from the asymptotic character of the series.

A well-known example of calculation of renormalization constants happens during the determination of the topological susceptibility in QCD or in CP$^{N-1}$ models. The Monte Carlo signal for this quantity is [1,2]

$$
\chi_{\text{latt}} = a^d(g_0)Z(g_0)^2\chi + a^d(g_0)A(g_0)\langle T \rangle_{NP} + P(g_0).
$$

(1.1)

In this equation $d$ is the space-time dimension, $a$ is the lattice spacing (related to the bare coupling through the beta function), $\langle T \rangle_{NP}$ is the non-perturbative part of the vacuum expectation value of the trace of the energy-momentum tensor and $Z(g_0)$, $A(g_0)$ and $P(g_0)$ are finite renormalizations. The topological susceptibility on the lattice is defined as

$$
\chi_{\text{latt}} = \frac{1}{V}\langle (Q_{\text{latt}})^2 \rangle,
$$

(1.2)

where $Q_{\text{latt}}$ is a suitable definition of the topological charge operator on the lattice and $V$ is the space-time volume.

The calculation of the constants $Z(g_0)$, $A(g_0)$ and $P(g_0)$ can be performed either by applying perturbation theory or by using the so-called heating method [3]. This is a direct non-perturbative method to evaluate the renormalization constants as it does not rely on any expansion. It consists in heating a classical initial configuration having a known topological charge $Q_0$. The previous renormalization constants will show up during the first steps of
thermalization because only short wave fluctuations are generated at this stage. This method has been used in the $O(3)$ non-linear $\sigma$-model \cite{3,4} and in QCD \cite{5}.

The aim of the present work is to check the validity of this non-perturbative method by comparing it with perturbation theory at large $\beta$ values. We performed the check on the $O(3)$ non-linear $\sigma$-model in two dimensions. In the continuum this model is defined by the action

$$S = \frac{1}{2g_0} \int d^2x (\partial_\mu \vec{\phi}(x))^2,$$

with the constraint $\vec{\phi}(x)^2 = 1$ for all $x$. On the lattice we will make use of the Symanzik tree-level improved action \cite{6}

$$S_{\text{latt}} = -\beta \sum_{x,\mu} \left( \frac{4}{3} \vec{\phi}(x) \cdot \vec{\phi}(x + \mu) - \frac{1}{12} \vec{\phi}(x) \cdot \vec{\phi}(x + 2\mu) \right).$$

Henceforth $\beta = 1/g_0$. The lattice definition we used for the topological charge density is

$$Q_{\text{latt}}(x) = \frac{1}{32\pi} \epsilon_{\mu\nu}\epsilon_{ijk} \phi^i(x) \left[ \phi^j(x + \mu) - \phi^j(x - \mu) \right] \left[ \phi^k(x + \nu) - \phi^k(x - \nu) \right].$$

The first two perturbative coefficients of $Z$ and $P$ for the previous lattice action and charge density are known \cite{3,4}. We will test the heating method by measuring these two renormalization constants at very large $\beta$.

At fixed lattice size $L$ and large $\beta$ all spins tend to be parallel and small fluctuations around the trivial vacuum is the only physics present in the system. The small value of the ratio $L/\xi(\beta)$ ($\xi$ is the correlation length) prevents disorder to appear. Therefore long wavelength fluctuations can hardly be generated. In these conditions perturbation theory becomes exact \cite{7}. On the other hand, within our statistical errors, the perturbative series can be well approximated by the first two coefficients if using $\beta = 100 \div 1000$. Hence this approximate result from the perturbative series should reproduce the obtained value from the heating method.

We chose the $O(3)$ non-linear $\sigma$-model because it is known that the instanton size distribution in this model favours small instantons \cite{8}. Therefore an instanton heated at $\beta = 1000$
can be well accommodated on a lattice size \( L \sim 1000a \) which is the biggest lattice we will use.

As a byproduct we show how to use the heating method to compute the first coefficients of the perturbative expansions in equation (1.1) with rather high precision.

In section 2 we will review the heating method and the results and conclusions will be shown in sections 3 and 4.

II. THE HEATING METHOD

The heating method \[3,9\] is a procedure to non-perturbatively determine the renormalization constants in equation (1.1). We start from a given classical configuration \( C_0 \) having some known topological charge \( Q_0 \). Then we construct ensembles of configurations \( \{C_n\} \) obtained after performing \( n \) thermalization steps on the initial \( C_0 \) configuration at some value of \( \beta \). For small \( n \) it is expected that the updating sweeps create only small fluctuations up to distances of a few lattice spacings. For this purpose it is important to use a slow updating algorithm. Convenient algorithms are Metropolis and heat-bath. We used a heat-bath algorithm. If the correlation length satisfies \( \xi(\beta) \gg a \) then we can assume that the configuration contains small statistical fluctuations on a background of topological charge \( Q_0 \). The main assumption of the method is that these fluctuations are responsible for the renormalizations \[3\]. Therefore if \( Q_0 = 1 \) and at each \( n \) we measure \( Q^\text{latt} \) then after few updating steps the measured value of \( Q \) divided by \( Q_0 \) will give us \( Z(\beta) \). If we measure \( \chi^\text{latt} \) and \( Q_0 = 0 \) then after few steps the Monte Carlo signal will reach the value of \( P(\beta) \).

To create the initial configuration \( C_0 \) with topological charge \( Q_0 = 0 \) we put all spins parallel to some axis. When the initial configuration must contain a charge \( Q_0 = 1 \) then we put by hand a charge-one instanton field on the lattice. For this purpose we use the well-known expression in the continuum for such one-instanton field \[10\],

\[
    w = \frac{z - z_0}{\rho \exp(i\theta)}; \quad w \equiv \frac{\phi^1 + i\phi^3}{1 - \phi^2},
\]

\[
(2.1)
\]
where \( z = x_1 + ix_2 \) is the coordinate on the two-dimensional euclidean space-time and \( z_0 \) is the center of the instanton; we always put this center at the geometrical center of the lattice, \( z_0 = (1 + i)L/2 \). In this equation \( \theta \) and \( \rho \) are the orientation and size of the instanton respectively. We chose \( \theta = \pi/4 \). In the next section we will discuss the value for \( \rho \). Once the instanton has been put on the lattice, we apply a relaxation process on the configuration to settle it. Indeed the initial charge is usually less than 1 and after the relaxation it approaches 1. The relaxation process is repeated until the value of \( Q_0 \) stabilizes.

The relaxation algorithm used was the cooling [11]. We performed 30 cooling steps.

However, even after the cooling, the background topological charge \( Q_0 \) was never exactly 1. It was close but less than 1. This fact is not surprising as there are no known exact instanton solutions on the lattice. Moreover it is known that a single topological charge-one field is not allowed on a continuum torus [12] and we use a periodic lattice to perform our numerical simulations. Therefore it is not clear whether the heating method to compute \( Z \) will work or not. In particular when we normalize the measured \( Q \) with \( Q_0 \), \( Z = Q/Q_0 \), we could use either the lattice non-integer value of \( Q_0 \) or the corresponding integer continuum value. Using exact toroidal biinstanton solutions [12] does not ameliorate the situation because on the lattice \( Q_0 \) is again close but less than 2. In this work we will try to clarify these points.

The signal of our observables measured during a numerical simulation is less noisy at large values of the ratio \( \xi/L \). In this case, we can get rather accurate results with low statistics. In particular, working at large values of \( \beta \) allows us to observe the lattice size dependence of the renormalization constants. We expect that the perturbative tail \( P \) have a clear dependence on \( L \) while the multiplicative renormalization might be independent of \( L \) as the perturbative procedure to obtain \( Z \) predicts.
III. SIMULATION AND RESULTS

In this section we will describe the simulations performed to determine both the multiplicative renormalization $Z$ and the perturbative tail $P$ in equation (1.1).

At large values of $\beta$ the signal from the mixing with the trace of the energy-momentum tensor (see equation 1.1) is totally negligible. Therefore we cannot check the perturbative expansion of $A$ in equation (1.1).

A. The multiplicative renormalization

We performed several measures of the multiplicative renormalization $Z(\beta)$. We used two lattices: $240^2$ with $\beta = 100$ and $1200^2$ with $\beta = 1000$. At these values of $\beta$ the ratio $\xi/L$ is $O(10^{100 \div 1000})$. In both cases we studied the dependence of the result on the instanton size $\rho$. The simulations showed a strong dependence on this parameter. For large instanton sizes $\rho/L \gtrsim 0.15$ the data raise while for small sizes $\rho \lesssim 8a$ the curve falls off (see Figure 1). In the first case finite lattice size effects distort the instanton distribution cutting it off at the boundary of the lattice. We understand that the Monte Carlo signal at these values of $\rho$ has no physical meaning. In the second case the instanton is too small and after few heating steps it gets dissolved in the statistical fluctuations around it. In consequence the topological content gets lost.

In between we see a window of instanton sizes for which the Monte Carlo signal of the heating method displays a long and clear plateau (see Figure 1). The value of $Z(\beta)$ is the height of the plateau normalized to the initial charge $Q_0$. The drift downwards of the curve for small $\rho$ makes it difficult to determine the value of $Z$. This fact is reflected in the larger error bars for small $\rho$. For large $\rho$ we chose the minimum of the curve as the value for $Z$. In Figure 2 and 3 we show the value of the plateau as a function of $\rho/L$ for the two lattices we used.

For values of $\beta$ in the scaling window of the model ($\beta \sim 1.5 \div 2.5$ in usual simulations)
a slow drop of the curves is seen. This is due to the creation of small size instantons with opposite charge than the initial one [13]. This is a systematic error which one has to face when applying the heating method to the $O(3)$ non-linear $\sigma$-model [14]. At large values of $\beta$, the strong critical slowing down prevents the creation of such instanton sea around the background. Hence we think that the behaviour of the data at small $\rho$ is well explained by the loss of the background instanton in the middle of the fluctuations.

Before extracting the value of $Z(\beta)$ from Figure 2 and 3 we will discuss the statistics used in each run. For the runs on a $240^2$ lattice at $\beta = 100$ we performed 1000 trajectories of 100 heating steps. The data shown in Figure 1 are the average of these 1000 trajectories. For the $1200^2$ lattice at $\beta = 1000$ we performed 20 trajectories of 150 heating steps. In each case an autocorrelation analysis was done. The data are correlated at distances of $\sim 5$ heating steps. We calculated the height and error of the plateau taking into account this effect. The step where the plateau starts can be determined by just having a look at the curve (see Figure 1). From this first point (say $n_0$) we averaged all heating steps until some $\bar{n}$, $n_0 < \bar{n} \leq 100$. The height of the plateau was obtained by looking for a stable result of this average while varying $\bar{n}$ from $n_0 + 1$ to 100.

The results of the calculation of $Z(\beta)$ for each $\rho$ are shown in Tables I and II corresponding to Figures 2 and 3 respectively. Getting the value of $Z(\beta = 1000)$ from Figure 3 is easy. The window of stable instanton sizes is apparent. As the lattice size diminishes, this window shrinks and becomes a flex point of the curve. To determine the flex point of the curve in Figure 2 we first interpolated the Monte Carlo points with an odd degree polynomial and then we evaluated analytically the flex point. Increasing the degree of the polynomial, the result for the flex stabilizes. In Table III we show the results of this calculation as a function of the degree of the interpolating polynomial.

The values for $Z(\beta)$ obtained from these figures are $Z(\beta = 100) = 0.993159(2)$ and $Z(\beta = 1000) = 0.999317(1)$. On the other hand the one-loop and two-loop order coefficients of this multiplicative renormalization are
\[ Z(\beta) = 1 + \frac{z_1}{\beta} + \frac{z_2}{\beta^2} + O\left(\frac{1}{\beta^3}\right) \quad z_1 = -0.684040, \quad z_2 = -0.0598. \quad (3.1) \]

The values for \( z_1 \) and \( z_2 \) were first calculated on finite size lattices by substituting the corresponding loop integrals for sums. Then these results were extrapolated to infinite lattice size. The extrapolating function was \( z_i(L) = z_i + \alpha / L^m \). This extrapolation was stable within ten digits for \( m = 2 \) without including logarithms of \( L \) in the previous function. Therefore the analytical prediction for the multiplicative renormalization is \( Z^{2\text{-loop}}(\beta = 100) = 0.993154 \) and \( Z^{2\text{-loop}}(\beta = 1000) = 0.999316 \). We see an excellent agreement between the theoretical and Monte Carlo values.

The lattice size independence of \( Z \) is hard to reveal from our method. To see a clear flex point in Figure 2 we must work on lattice sizes satisfying \( 8a \lesssim 0.15L \) which means \( L \gtrsim 60a \). At \( L = 60a \) the difference \( |z_1 - z_1(L = 60a)| \sim 10^{-4} \) cannot be seen at the values of \( \beta \) we work.

All the data shown for \( Z \) were equal to the Monte Carlo signal for \( Q \) divided by the initial charge on the lattice after 30 cooling steps, \( Q_0 \). We could also divide \( Q \) by the corresponding continuum initial charge, \( i.e. \): the integer closest to the lattice value of \( Q_0 \). The lattice values of \( Q_0 \) are \( Q_0 = 0.99901 \) on the \( 240^2 \) lattice at \( \rho/L = 0.11 \) and \( Q_0 = 0.99981 \) on the \( 1200^2 \) lattice at \( \rho/L = 0.05 \). Notice that these values cannot depend on \( \beta \). The corresponding continuum values would clearly be \( Q_0 = 1 \). Had we used these continuum values for normalizing the Monte Carlo signal we would have got wrong results for \( Z \). Indeed for the \( 240^2 \) lattice at \( \beta = 100 \) we would have obtained 0.992176(2) while for the \( 1200^2 \) lattice at \( \beta = 1000 \) the result would have been 0.999127(1). We conclude that the normalization has to be done by consistently using the lattice value of \( Q_0 \).

We can also look at the problem the other way round and try to determine the value of \( z_1 \) from the Monte Carlo data. Equating the Monte Carlo value for \( Z(\beta = 1000) \) to \( 1 + z_1/1000 \) we get \( z_1 = -0.683(1) \). We can do the same for \( Z(\beta = 100) \) obtaining \( z_1 = -0.6841(2) \). These results are in agreement with equation (3.1).
B. The perturbative tail

The determination of the perturbative tail $P$ can be performed by heating a trivial configuration, \textit{i.e.:} all spins parallel to some previously chosen direction $\vec{v}$ in the $O(3)$ space. We started every trajectory with a different direction $\vec{v}$ chosen at random. We used rather small lattices in order to check the lattice size dependence of $P$: $L = 9a$ and $L = 48a$.

The dashed line and circles in Figure 4 display the perturbative prediction and the result of the simulation on a $9^2$ lattice at $\beta = 100$. We performed 60 heating steps and $10^4$ trajectories. The perturbative tail has the form

$$P(\beta) = \frac{p_4}{\beta^4} + \frac{p_5}{\beta^5} + O(\frac{1}{\beta^6}).$$

At $L = 9a$ the values of the coefficients are $p_4 = 6.036 \times 10^{-5}$ and $p_5 = 5.159 \times 10^{-5}$. To calculate the second coefficient we must include the zero mode contribution which amounts to $\sim 7\%$ of the whole term. Hence $P^{1\text{-loop}}(\beta = 100, L = 9a) = 6.088 \times 10^{-13}$. In Figure 4 we see an impressive agreement with the Monte Carlo value $P(\beta = 100, L = 9a) = 6.09(3) \times 10^{-13}$. In doing the fit to an horizontal line we eliminated the autocorrelations of the data.

The solid line and triangles in Figure 4 display the same perturbative prediction and simulation for a $48^2$ lattice. Each trajectory consisted of 100 heating steps. For this lattice size the perturbative coefficients are $p_4 = 6.804 \times 10^{-5}$ and $p_5 = 5.722 \times 10^{-5}$. Here the zero mode term is negligible. Therefore $P^{1\text{-loop}}(\beta = 100, L = 48a) = 6.861 \times 10^{-13}$. The Monte Carlo result is $P(\beta = 100, L = 48a) = 6.85(2) \times 10^{-13}$. The agreement is again satisfactory. We can see a lattice size dependence in the perturbative tail which agrees with the one predicted by perturbation theory.

Again we can compute the first perturbative coefficients from the previous Monte Carlo data. From the data on a $9^2$ lattice and neglecting the contribution at four loops, we get $p_4 = 6.09(3) \times 10^{-5}$. On $48^2$ we get $p_4 = 6.85(2) \times 10^{-5}$. 
IV. CONCLUSIONS

In this work we have checked the heating method to calculate the renormalization constants present in the determination of the topological susceptibility on the lattice. We simulated the $O(3)$ non-linear $\sigma$-model in two dimensions. We used the method at large correlation lengths in order to eliminate all non-perturbative effects and see only the perturbation-theory predictions on the Monte Carlo signal. The idea is based on the fact that at fixed lattice size $L$ and large correlation lengths $\xi/L \to \infty$ perturbative calculations are expected to become exact. This conjecture has been rigorously proven in the $XY$ model [7]. The positive conclusion of the test we performed supports the conjecture also on the $O(3)$ model.

The choice of the $O(3)$ $\sigma$-model was motivated by the fact that this model can accommodate small instantons [8] and at very large correlation length the size of the lattice in physical units strongly diminishes.

We computed the multiplicative renormalization $Z$ of the lattice topological charge, $Q_{\text{latt}} = QZ$ as well as the perturbative tail of the corresponding topological susceptibility $P$. Hence we computed static quantities by using a Monte Carlo simulation thus proving that the renormalization effects are the average of the statistical fluctuations.

Concerning the calculation of the multiplicative renormalization $Z$ we know that one-instanton solutions do not exist on the lattice and they are absent even for continuum tori [12]. However we have checked that the usual solutions on the continuum space-time [10] can be used to calculate $Z$ even though they present a non-integer topological charge and are not stable solutions of the lattice field equations. We think that this is a notable result.

Other conclusions which come out from our computation of $Z$ are (i) the background charge $Q_0$ remains stable during the whole heating trajectory, indeed we showed that the final result for $Z$ is quite sensitive to the value of $Q_0$; (ii) we see that although small fluctuations soon raise, small instantonic objects which could lower the value of $Z$ are absent, thus the critical slowing down seems to apply also to small instantons.
Another clear conclusion of this work is that to compute $Z$ we must always divide the Monte Carlo signal $Q$ by the non-integer lattice topological charge $Q_0$ of the initial configuration.

A natural question raises at this point: does the $\rho$ dependence persist at values of $\beta$ in the scaling window ($\beta \sim 1.5 \div 2.5$)? At low values of $\beta$ there is more disorder in the configuration resulting in larger statistical fluctuations which bring about larger error bars in the lattice measure of any observable. On the other hand small topological objects can appear yielding a modification of the trajectories. Therefore the answer of the previous question is possibly yes but the largest statistical and systematic errors overwhelms this effect.

Finally, concerning the calculation of the perturbative tail, we saw a good agreement between perturbation theory and Monte Carlo results. They also displayed a lattice size dependence according to the perturbation-theory predictions.

The heating method works well and when correctly used it gives the right answers. One has to take care also to the point where the plateau sets in (in our simulations it sets in after many heating steps, about 40 for the multiplicative renormalization) and also to the strong autocorrelations which can mask the true plateau.

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Figure captions

Figure 1. Monte Carlo signal for the topological charge after 100 heat-bath sweeps on a one instanton background field. A lattice size $L = 240a$ and $\beta = 100$ was used. The lower trajectory corresponds to $\rho = 0.05L$ (down triangles), the trajectory in the middle is for $\rho = 0.13L$ (rectangles) and the upper curve is for $\rho = 0.19L$ (up triangles). A similar figure is obtained for the other lattice size used, $L = 1200a$.

Figure 2. Values obtained for $Z$ on a $L = 240a$ lattice and $\beta = 100$ as a function of the instanton size over $L$. The solid line is to guide the eye. The dashed line is the 2-loop value.

Figure 3. Values obtained for $Z$ on a $L = 1200a$ lattice and $\beta = 1000$ as a function of the instanton size over $L$. The solid line is to guide the eye. The dashed line is the 2-loop value.

Figure 4. Monte Carlo signal of the topological susceptibility at $\beta = 100$. Triangles and solid line (circles and dashed line) are the Monte Carlo signal and perturbative prediction on a $48^2$ ($9^2$) lattice. On the $48^2$ ($9^2$) lattice, 100 (60) heat-bath sweeps were performed.

Table captions

Table I. Values of $Z$ as a function of the instanton size $\rho/L$. Results of a lattice size $L = 240a$ and $\beta = 100$.

Table II. Values of $Z$ as a function of the instanton size $\rho/L$. Results of a lattice size $L = 1200a$ and $\beta = 1000$.

Table III. Flex point $\zeta$ obtained in the interpolation with a polynomial of degree $p$. The interpolation was performed on the data of Table I.
Table I

| $\rho/L$ | $Z(\beta = 100)$     |
|----------|----------------------|
| 0.03     | 0.993019(6)          |
| 0.05     | 0.993094(2)          |
| 0.07     | 0.993144(2)          |
| 0.09     | 0.993156(1)          |
| 0.11     | 0.993178(1)          |
| 0.13     | 0.993201(1)          |
| 0.15     | 0.993234(1)          |
| 0.17     | 0.993270(1)          |
| 0.19     | 0.993317(1)          |
| 0.21     | 0.993369(1)          |

Table II
| $\rho/L$ | $Z(\beta = 1000)$          |
|---------|---------------------------|
| 0.005   | 0.999267(10)             |
| 0.007   | 0.999311(6)              |
| 0.01    | 0.999318(3)              |
| 0.03    | 0.999317(1)              |
| 0.05    | 0.999317(1)              |
| 0.07    | 0.999319(1)              |
| 0.09    | 0.999323(1)              |
| 0.11    | 0.999330(1)              |
| 0.13    | 0.999344(1)              |
| 0.15    | 0.999366(1)              |
| 0.17    | 0.999398(1)              |
| 0.19    | 0.999440(1)              |
| 0.21    | 0.999501(1)              |

**Table III**

| $p$ | $\zeta$ |
|-----|---------|
| 3   | 0.993197 |
| 5   | 0.993162 |
| 7   | 0.993154 |
| 9   | 0.993159 |
Figure 1

![Graph showing the relationship between heating step and $Q/Q_0$.](image-url)
Figure 2

![Graph showing the relationship between \( \rho / L \) and \( Z(\beta=100) \)]
Figure 3

$Z(\beta=1000)$ vs $\rho/L$
