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DISLOCATIONS AND TOPOLOGICAL BACKGROUND IN
THE LATTICE $O(3)$ σ MODEL

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ABSTRACT

Dislocations are identified to be responsible for the anomalous scaling behaviour of the topological susceptibility in the lattice $O(3)$ σ model. The results are based on a numerical investigation. For $1.9 \geq \beta \geq 1.7$ Monte Carlo data for a topological background susceptibility are consistent with weak coupling renormalization group scaling.

In a previous article¹⁾ the topological charge Q was defined for the lattice $O(3)$ σ model and Monte Carlo (MC) results were presented for the topological susceptibility

$$\chi_t = \langle Q^2 \rangle / V \quad (V = \text{Volume}) \quad (1)$$

The scaling behaviour

$$\chi_t = \frac{\text{const}}{a^2} \cdot \beta^2 \cdot \exp(-\alpha \cdot \beta), \quad \alpha = 4\pi \quad (2)$$

was expected for large β . The MC investigation, however, revealed $\alpha \approx 2.5\pi = 7.85\dots$. The result has been confirmed by Martinelli et al.²⁾

In this note I present a closer inspection of the MC contribution to the topological charge. Some of the results overlap with conclusions from analytic considerations by Lüscher³⁾. To keep this letter self-contained, let me first introduce the notation and define the topological charge on the lattice. For details consult Ref. 1).

The action of the lattice $O(3)$ σ model is given by

$$S = \sum_{\langle i, j \rangle} (1 - \vec{s}_i \cdot \vec{s}_j), \quad i = (i_1, i_2), \quad j = (j_1, j_2) \quad (3)$$

The sum goes over nearest neighbours on a two-dimensional lattice Λ , which is supposed to be a triangular or a square lattice with lattice spacing a on a torus. The three-dimensional spins are normalized to $\vec{s}_j^2 = 1$, i.e., they lie on the sphere S_2 and can be parametrized by polar and azimuthal angles δ and φ . Vacuum expectation values of operators are given by

$$\langle O \rangle = Z^{-1} \int \prod_{i \in \Lambda} \pi d\vec{s}_i \cdot O\{\vec{s}_i\} \cdot \exp(-\beta S\{\vec{s}_i\}) \quad (4)$$

with

$$\int d\vec{s} = \frac{1}{4\pi} \int_{-1}^1 d\cos\vartheta \int_0^{2\pi} d\varphi \quad \text{for} \quad \vec{s} = \vec{s}(\vartheta, \varphi)$$

The partition function Z normalizes $\langle 1 \rangle = 1$.

Let me first consider a triangular lattice. The triangles can be labelled by points j^* on the lattice Λ^* . To each triangle three spins are attached. Up to certain exceptional configurations [of measure zero in (4)] three spins $\vec{s}_1, \vec{s}_2, \vec{s}_3$ on the sphere S_2 uniquely define a minimal spherical triangle with angles $\alpha_1, \alpha_2, \alpha_3$. Its area is given by

$$A = \alpha_1 + \alpha_2 + \alpha_3 - \pi \quad (5)$$

By elementary geometry the angles are related to the spin vectors. For instance

$$\alpha_3 = \arccos \left(\frac{\vec{a}_1 \cdot \vec{a}_2}{|\vec{a}_1| |\vec{a}_2|} \right) \quad (6)$$

where

$$\vec{a}_1 = \frac{\vec{\lambda}_1}{\vec{\lambda}_1 \cdot \vec{\lambda}_3} - \vec{\lambda}_3 \quad \text{and} \quad \vec{a}_2 = \frac{\vec{\lambda}_2}{\vec{\lambda}_2 \cdot \vec{\lambda}_3} - \vec{\lambda}_3$$

The signed area is $A_\sigma(\vec{s}_1, \vec{s}_2, \vec{s}_3) = \sigma \cdot A$, $\sigma = \text{sign}[\vec{s}_1(\vec{s}_2 \times \vec{s}_3)]$. With the definition

$$q(x^*) = \frac{1}{4\pi} A_\sigma(\vec{\lambda}_1, \vec{\lambda}_2, \vec{\lambda}_3)$$

of the topological charge density, the topological charge

$$Q = \sum_{x^* \in \Lambda^*} q(x^*)$$

takes integer values $0, \pm 1, \dots$, because the signed areas can only add up to zero or wind one or several times (in a positive or negative direction) around the sphere.

In the following I always consider a square lattice. For the square lattice there are two equally good definitions of the topological charge. Let j^* again be a vertex of the dual lattice, which labels the plaquette, and the spins $\vec{s}_1, \vec{s}_2, \vec{s}_3, \vec{s}_4$ be attached in anticlockwise direction to the corners of the plaquette. According to the two possibilities of dividing the square into triangles the definitions of the topological charge are

$$q_1(x^*) = \frac{1}{4\pi} \{ A_\sigma(\vec{\lambda}_1, \vec{\lambda}_2, \vec{\lambda}_4) + A_\sigma(\vec{\lambda}_3, \vec{\lambda}_4, \vec{\lambda}_2) \} \quad (7a)$$

and

$$q_2(x^*) = \frac{1}{4\pi} \{ A_\sigma(\vec{\lambda}_2, \vec{\lambda}_3, \vec{\lambda}_1) + A_\sigma(\vec{\lambda}_4, \vec{\lambda}_1, \vec{\lambda}_3) \} \quad (7b)$$

For fields with small action $q_1(x^*) = q_2(x^*)$. Otherwise $q_1(x^*) - q_2(x^*) = 0, \pm 1$ is possible.

By considering topologically non-trivial configurations one thinks, of course, immediately about instantons. For the continuum theory instantons of topological charge $K = \pm 1, \pm 2, \dots$, and action $4\pi |K|$ are regular solutions of the Euclidean field equations and minima of the classical action⁴⁾.

For smooth field configurations the topological charge density on the lattice approaches the corresponding continuum density in the classical limit $a \rightarrow 0$. I have studied finite size effects of the lattice by measuring the topological charge Q and the total action S of multi-instanton solutions in the parametrization

$$W = \left\{ \sum_{i=1}^K \frac{\rho_i}{z - r_i} \right\}^{-1} \quad (8)$$

on a 100^2 lattice. Here $w = w_1 + iw_2$ are stereographic co-ordinates of the field $\vec{s} = \vec{s}(x, y)$, $z = x + iy$. r_i are positions and ρ_i are (complex) scale size parameters. The lattice sites are labelled by $(n, m) = (0, 0) \dots (99, 99)$.

For a reasonable choice of the parameters ($99 \gg |r_i - r_j| \gg |\rho_i| + |\rho_j| \gg 1$, lattice spacing $a=1$) instantons of the continuum theory give rise to configurations of non-zero topological charge on the lattice, which are quasistable under the transformation

$$\vec{\lambda} \rightarrow \frac{\vec{s}}{|\vec{s}|}, \quad \vec{s} = \sum_{i=1}^4 \vec{\lambda}_i \quad (\vec{s}_i = \text{nearest neighbours of } \vec{s}) \quad (9)$$

which transforms the spin $\vec{s}$ on the lattice into its local minimum with respect to the action (3).

What is meant by quasistable becomes obvious from Fig. 1, where the action and topological charge of a one instanton solution dependent on a number of iterations (altogether 1300) with the transformation (9) is plotted. [One iteration is defined by applying (9) to each spin of the lattice once.] Figure 2 gives action and topological charge of a one-instanton solution on the lattice as

function of $|\rho|$ before and after one iteration with (9). It is clear that the dilatation invariance is broken by the lattice. The instanton represented in Fig. 1 shrinks under iterations with (9) until it has become a "dislocation" (at step 920) and is then annihilated. Finally Table 1 summarizes values for multi-instanton solutions with $\rho_j = 3 + i3$ and $r_j = (14.5 + 25 \cdot j) \bmod 100 + i(14.5 + 25 \cdot [\frac{j}{5}])$. In the following I call a topologically non-zero configuration on the lattice quasistable if it does not change its topological charge under at least one iteration with the transformation (9).

MC simulations approximate the integral (4) over all configurations by "importance sampling"⁵⁾. The heat bath method selects the new spin $\vec{s}$ dependent on its nearest neighbours with a weight proportional to

$$d\gamma \cdot d\alpha \cdot \exp(-\beta \cdot |\vec{s}| \cdot |\vec{S}| \cdot \cos \alpha) \quad (10)$$

Here $\alpha = \angle(\vec{s}, \vec{S})$ and γ is an angle in the plane orthogonal to $\vec{S}$. A sweep is an iteration with (10) through the lattice. On a finite lattice a sweep goes over into an iteration with (9) for $\beta \rightarrow \infty$. This is not true in the continuum quantum field theoretical limit $\beta \rightarrow \infty$, because in this limit the physical length scale is set by the correlation length ξ and

$$\xi = a \cdot \text{const} \cdot \beta^{-1} \exp(+2\pi\beta) \quad \text{for} \quad \beta \rightarrow \infty$$

That is to say, the number of plaquettes in any area of physical magnitude increases exponentially.

In Ref. 1) we have performed a MC measurement of the magnetic susceptibility χ_m and the topological susceptibility χ_t on a 100^2 lattice. The scaling region $1.3 \leq \beta \leq 1.7$ roughly (with about 20% error bars) corresponds⁶⁾ to $4 \leq \xi \leq 32$. For the magnetic susceptibility a deviation from the scaling law was found of an order of magnitude, which allows an explanation by higher order perturbative corrections, in agreement with Ref. 7). The topological susceptibility, however, failed the scaling law completely and $\alpha \approx 2.5\pi$ instead of $\alpha = 4\pi$ in (2) was obtained.

Let me distinguish two possible contributions to the topological charge Q . A dislocation is a non-zero contribution to the topological charge, which comes from a region G with area $A(G) \rightarrow 0$ for $\beta \rightarrow \infty$ (i.e., the charge density develops a singularity). A contribution to the topological charge, which comes from a region G with finite area $A(G)$ for $\beta \rightarrow \infty$, is called a topological background configuration (i.e., the charge density is supposed to converge against a continuous function).

In the instanton picture one considers quantum fluctuations around classical minima of the action of non-zero topological charge. In a MC simulation with large enough β and a large enough lattice this corresponds to quasistable topological background contributions. For two successive MC sweeps contributions of this type are strongly correlated.

On the other hand, dislocations are strongly peaked local maxima of the action and therefore unstable under iterations with the transformation (9). The probability to find a dislocation around a certain plaquette decreases exponentially with $\beta \cdot S_d$ for $\beta \rightarrow \infty$, where S_d is the action of the dislocation. As the number of plaquettes increases exponentially with $4\pi\beta$ for $\beta \rightarrow \infty$ in any region of physical size, it follows that dislocations can give in the continuum limit a relevant contribution to the topological charge if their minimal action is less than 4π . In a MC simulation dislocations of two successive sweeps are expected to be uncorrelated.

A special example for dislocations are plaquettes with $q_1(x^*) \neq q_2(x^*)$ [cf. Eq. (7)]. They are called special one plaquette (SOP) dislocation in the following. In the MC simulation¹⁾ the topological charges Q_1, Q_2 were measured according to the definitions (7a) and (7b). Within the statistical errors we had

$$\langle Q^2 \rangle \stackrel{\text{def}}{=} \frac{1}{2} \langle Q_1^2 + Q_2^2 \rangle = \langle Q_1^2 \rangle = \langle Q_2^2 \rangle$$

The results for Q_1 and Q_2 , however, turned out to be different for most (e.g., for 82% at $\beta = 1.7$) of the measurements in the considered region of β . A more detailed investigation of the topological charge density revealed that many SOP dislocations contribute to the topological charge. Figures 3a and 3b give the positions of SOP dislocations for two successive sweeps at $\beta = 1.7$ on a 100^2 lattice in equilibrium. No correlations between positions in successive sweeps were observed. It turns out that $\langle (Q_1 - Q_2)^2 \rangle$ scales with the same power as $\langle Q^2 \rangle$. Even more remarkable, up to small deviations (comparable in order of magnitude to the statistical fluctuations) $\langle (Q_1 - Q_2)^2 \rangle = \langle Q^2 \rangle$ was found.

Using the transformation (9) I have performed a MC investigation on a 100^2 lattice which tries to separate the contributions from dislocations and a possible quasistable topological background to χ_t . More precisely: after each MC sweep I have iterated n times ($n=1,2,\dots$) with the transformation (9), where n was determined from the condition

$$Q_b \stackrel{\text{def}}{=} Q_1(n) = Q_2(n) = Q_1(n-1) = Q_2(n-1)$$

This procedure is rather time consuming, since after each iteration with (9) the topological charge has to be measured, and the results presented here are somewhat preliminary.

Let us call Q_b topological background charge and define topological dislocation charges as

$$Q_{\hat{a}} = Q_i - Q_a \text{ and } (\hat{a} = 1, 2).$$

The corresponding susceptibilities are

$$\chi_b = \langle Q_b^2 \rangle / V \quad \chi_a = \frac{1}{2V} (\langle (Q_a^1)^2 + (Q_a^2)^2 \rangle),$$

and topological defects are defined by

$$\delta_a = 10^4 \cdot \lambda^{4\pi(\beta-1.3)} \cdot \chi_a \quad (a = t, b, a).$$

For $\beta \rightarrow \infty$ (on a very large lattice) dislocations become more and more dilute in units $[a]$ of the lattice spacing and they are expected to be eliminated by few iterations with (9). A quasistable topological background, which extends over many lattice spacings, is left unchanged. For instance also an instanton of arbitrary small scale size $|\rho|$ extends over a region of many plaquettes in the limit $\beta \rightarrow \infty$; $\rho =$ fixed in units of $[\xi]$.

For small β the spins are barely correlated and the dislocations are not well separated. In this case the charge Q_b is generated by many iterations with (9). Then Q_b has nothing to do with a quasistable topological background, but is essentially a random charge, depending only on artifacts of the configuration to which the iterations with (9) are applied. For a random charge Q_b one has

$$\chi_c \stackrel{\text{def}}{=} \langle Q_a \cdot Q_b \rangle / V = -\chi_b,$$

whereas in the case of a well-defined topological background, one has $\chi_c = 0$. Therefore I take $(-\chi_c)/\chi_b$ as a measure for the randomness of the generated background charge Q_b . Table 2 summarizes the MC data. At each value of β 7200 or more sweeps were done first for taking the lattice to equilibrium. We see that $(-\chi_c)/\chi_b$ decreases from 0.44 to 0.11 in the region $1.3 \leq \beta \leq 1.8$.

Another feature of a well-defined background charge is that we expect correlations over several sweeps. Under omission of the charge zero sectors we compare in Fig. 4 the average length of groups of successive sweeps with constant charge for Q_i ($i=1,2$) and Q_b . For $\beta \geq 1.7$ the charges of successive sweeps are seen to be strongly correlated. At $\beta = 2.1$ the statistics is very poor since 98% of the configurations were found in the $Q_b = 0$ sector.

The topological defects are plotted in Fig. 5. The susceptibility χ_d of dislocations scales with the same coefficient $\alpha \approx 2.5\pi$ as χ_t . For $1.9 \geq \beta \geq 1.7$ the MC data for the topological background susceptibility χ_b are consistent with weak coupling renormalization group scaling ($\alpha \approx 4\pi$). They are, however, not yet completely convincing because of two reasons: 1) The error bars are large and 2) the correlation length is presumably already large compared with the lattice spacing. Using available more advanced computer techniques one can increase the lattice size and improve the statistics. Whether the topological background charge is related to any kind of instanton picture also requires further investigation.

I have estimated the scaling coefficient α [cf.(2)] by a MC calculation of the mean action $\bar{S}_d$ of dislocations caused by a few plaquettes embedded in a fixed background. In the scaling region the lowest average action had roughly the numerical value $\bar{S}_d \approx 10$ and was obtained by varying only the spins of one plaquette.

The dilute ansatz for dislocations implies for very large β : $\alpha \rightarrow S_d$, where S_d is the minimal action of dislocations. The mean action $\bar{S}_d \approx 10$ is significantly larger than the minimal action of Ref. 3). This means that entropy arguments for dislocations still play a significant role in the considered scaling region. In view of a rather large background action (e.g., mean action/link ≈ 0.34 at $\beta = 1.7$), one can argue that in the scaling region $\alpha \approx (\bar{S}_d - \bar{S})$, where $\bar{S}$ is the mean action for the links, which make the dislocation. The obtained values fit very well $\alpha \approx 2.5\pi$.

Dislocations are small scale fluctuations, in which one is not interested in the continuum quantum field theory limit. If we group spins together to block spins (e.g., square blocks BL of fixed size)

$$\vec{s}_{BL} = \frac{\sum_{i \in BL} \vec{s}_i}{\left| \sum_{i \in BL} \vec{s}_i \right|}$$

and apply the definition of the topological charge to the block spin $\vec{s}_{BL}$, then this gives rise to a topological charge Q_{BL} , which is well defined in the sense that Q_{BL} still assumes integer values and reduces to the winding number in the

classical continuum limit. That is to say, there is an infinite number of definitions of the topological charge on an equivalent footing. Therefore, another point of view on dislocation and topological background is provided by combining the definition of the topological charge with the MC renormalization group (MCRG). In a MCRG calculation [cf. Ref. 6) for the present model] the short distance fluctuations are integrated out and in the case of the topological charge, the calculation would be only sensitive with respect to the topological background. Even more simple: as the minimal action of a dislocation is > 0 , it follows that one can eliminate all dislocations by one single transformation which groups spins together to (large enough) blocks, before measuring the topological charge. This definition of the topological charge would still take into account instantons of arbitrary small scale size (which are in my notation different from dislocations). The ultra-violet divergence of the one instanton scale size integration in the $O(3)$ σ model requires an additional cut-off of fixed physical size at small distances. Results on this approach will be published elsewhere.

In summary: dislocations explain the anomalous scaling of the topological susceptibility. For large β dislocations and quasistable topological background separate clearly and the scaling law for the topological background susceptibility χ_b is consistent with weak coupling renormalization group. By grouping spins into blocks definitions of the topological charge are possible, which avoid the problem of dislocations from the beginning.

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Table 1

K	S	Q	S_1	S_2
1	12.6	1	25.5	13.2
2	25.1	2	62.7	27.2
4	50.3	4	152	56.6
8	101	8	335	119
10	126	10	408	151
11	138	10	435	164
12	151	11	458	177
14	176	12	495	200
16	201	15	519	217

Multi-instanton solutions on the lattice: K = charge in the continuum, S = action in the continuum, Q = measured charge (identical before and after the iterations), S_1 = action on the lattice, S_2 = action on the lattice after 24 iterations with (9).

Table 2

β	$X_t \cdot 10^4$	$X_d \cdot 10^4$	$X_b \cdot 10^4$	$(-X_c)/X_b$	$\bar{n}$	$Q_b = 0$	Sweeps
1.3	63.3 ± 1.7	61.3 ± 2.3	14.3 ± 0.9	$0.37 - 0.5$	4.7	10%	2000
1.5	22.7 ± 0.5	20.8 ± 0.4	6.2 ± 0.3	$0.31 - 0.39$	3.4	17%	2400
1.7	6.2 ± 0.4	4.9 ± 0.1	1.8 ± 0.5	$0.09 - 0.21$	2.3	35%	2400
1.8	2.66 ± 0.10	2.29 ± 0.06	0.46 ± 0.06	$0.06 - 0.15$	2.0	66%	3600
1.9	1.13 ± 0.06	1.03 ± 0.03	0.13 ± 0.05	$0.07 - 0.19$	1.8	88%	4800
2.1	0.256 ± 0.007	0.240 ± 0.007	0.018 ± 0.003	$-0.002 - 0.1$	1.3	98%	3600

MC data: the susceptibilities X_t , X_d , X_b and $(-X_c)/X_b$, the average number $\bar{n}$ of iterations with (9) per MC sweep, the contribution of the $Q_b = 0$ sector in per cent of the sweeps and the number of sweeps.

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FIGURE CAPTIONS

Fig. 1 : Action of a one instanton solution under 1300 iterations with transformation (9) on a 100^2 lattice.

Fig. 2 : Action and topological charge for the one instanton solution on the lattice (dependent on the scale size $|\rho|$) before and after one iteration with (9). Position: $r = 49.5 + i \cdot 49.5$ and scale size: $\rho = |\rho|$.

Fig. 3 : Positions of SOP dislocations for two successive sweeps at $\beta = 1.7$.

Fig. 4 : Average length of groups with constant non-zero charge Q_i ($i=1,2$): x and Q_b : $\bullet$.

Fig. 5 : Topological defects: $\delta_t \vec{t}$, $\delta_d \vec{d}$ and $\delta_b \vec{b}$.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5