Scaling and θ Dependence in the O(3) σ Model

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We use Monte Carlo simulations to examine the θ dependence of the O(3) σ model. The free energy as a function of θ is determined and its peculiar scaling properties are clarified.

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There has been considerable interest in the subject of topology on the lattice in recent years.[1-7] In particular, it has been shown that meaningful Monte Carlo simulations can be performed at nonzero values of the vacuum angle θ.[6] In this paper we consider some aspects of the topological charge in the (Euclidean) O(3) nonlinear σ model in two dimensions.[1,3,8] Apart from being interesting in its own right, at nonzero θ this model may be relevant in the understanding of the quantized Hall effect.[9]

The dynamical variables in the O(3) model are three-dimensional unit vectors n^a $(a=1,2,3)$ with the continuum action

$$S=\tfrac{1}{2}\int d^2x\,[\partial_\mu n^a(x)]^2. \tag{1}$$

For a finite system with periodic boundary conditions, the configuration $n^a(x)$ defines a mapping from the two-torus T_2 onto $O(3)/O(2)=S_2$. Since $\Pi_2(S_2)=Z$, the model exhibits nontrivial topology. The topological charge

$$Q=\frac{1}{8\pi}\int d^2x\,\epsilon_{\mu\nu}\epsilon_{abc}\,n^a(\partial_\mu n^b)(\partial_\nu n^c) \tag{2}$$

is the winding number of the mapping, and is always an integer. The partition function of the model depends on the vacuum angle θ:

$$Z(\theta,\beta)=\int Dn\; e^{(-\beta S+i\theta Q)}. \tag{3}$$

One can also define a lattice version of this model. A popular lattice action is

$$S=-\sum_{i,\mu,a} n^a(i)\,n^a(i+\mu). \tag{4}$$

The variables $n^a(i)$ are defined on the sites of the lattice. To add a θ term to this action, one must have a definition for the topological charge of a given lattice configuration. In contrast to the case of the four-dimensional gauge theory, in the O(3) model, the definition of Q is straightforward.[1] In our numerical simulations, motivated by Ref. 5, we compute Q as follows: First, the lattice is divided into triangles by bisecting each unit plaquette. These triangles are mapped into oriented spherical triangles in S_2 by the fields $n^a(i)$. The topological charge is given by the number of times these spherical triangles cover a reference point on S_2 (say the north pole).

One important difference between the four-dimensional gauge theory and the O(3) σ model will play a crucial role in the following discussion. If one computes the free energy per unit volume $F(\theta,\beta)=-V^{-1}[\ln Z(\theta,\beta)-\ln Z(0,\beta)]$ (the vacuum energy density) in the dilute-gas approximation, one finds an ultraviolet divergence in the continuum limit. It arises from a divergence in the integration over instanton scale sizes ρ from small sized instantons.[3,8] As a consequence of this, the topological susceptibility on the lattice,

$$\chi(\beta)=\langle Q^2\rangle/V=\partial^2F(\theta=0,\beta)/\partial\theta^2, \tag{5}$$

which suffers from the same uv divergence, does not scale in the continuum limit.[1,3] This divergence occurs because of the condensation of instantons for which $\xi \gg \rho$ (ξ is the correlation length). This is not a lattice artifact and cannot be "cured."[1,3] The divergence on the lattice is not as mild as in the continuum computation where it is only logarithmic.

Note that even in the four-dimensional gauge theory and in $CP^{(n-1)}$ models in two dimensions with $n>2$, χ may not scale for some definitions of Q on the lattice or for certain choices of the lattice action.[4,7] In this case, however, the divergence comes from instantons of scale size ρ of the order of the lattice spacing a which condense into the vacuum in the continuum limit and give a divergent χ. This effect is a lattice artifact and can be avoided either by a modification of the lattice action or by adopting a more restrictive definition for the topological charge.[4,7]

Since $F(\theta,\beta)$ is an even periodic function of θ, it can be expanded in a Fourier cosine series;

$$F(\theta,\beta)=\sum_{n=1}^{\infty} a_n(\beta)(1-\cos n\theta). \qquad (6)$$

In the dilute-gas approximation, all the coefficients except a_1 vanish. The higher harmonics (a_n, $n>1$) are related to deviations from the dilute-gas approximation. They represent interactions between instantons which occur when the gas is not dilute. The uv divergence in the continuum limit of $F(\theta,\beta)$ means that although

$$F(\theta,\infty)=0, \qquad (7)$$

$$\xi^2(\beta)F(\theta,\beta)\sim\beta^{-2}e^{4\pi\beta}F(\theta,\beta)\to\infty, \quad \text{as } \beta\to\infty. \qquad (8)$$

This divergence is a result of instantons with scale size $a \ll \rho \ll \xi$. Their number per physical volume $[\xi^2(\beta)]$, diverges as $\beta\to\infty$. On the other hand, their number per unit volume, in lattice units, goes to zero in the continuum limit. The ratio between their size and their average separation, which is a measure of their interaction, vanishes in the continuum limit. Therefore, the instantons that cause the uv divergence are dilute and their effect should be well described in the dilute-gas picture. One then expects that the uv divergence is present only in the coefficient a_1 in Eq. (6). All higher harmonics ($a_n, n>1$) should be free of uv divergences and should scale in the continuum limit. We note here that this statement about the uv divergence in F being present only in the coefficient of the $\cos\theta$ term is also implicit in a recent paper of David.[10] The arguments given above motivate the conjecture:

$$a_n(\beta)\to c_n e^{-4\pi\beta}\beta^2, \quad \beta\to\infty \text{ for } n\geq 2. \qquad (9)$$

An immediate consequence of this conjecture is that for large β, $F(\theta,\beta)$ is dominated by the first harmonic term $a_1(\beta)(1-\cos\theta)$. Therefore, any nonanalytic structure in $F(\theta,\beta)$, signaling a phase transition, becomes more difficult to determine numerically for large β, i.e., near the continuum limit.

One simple way to verify Eq. (9) is to study the scaling properties of

$$\begin{aligned} G(\beta) &= \frac{1}{V}(\langle Q^2\rangle_c-\langle Q^4\rangle_c), \\ &= \partial^2F(\theta=0,\beta)/\partial\theta^2+\partial^4F(\theta=0,\beta)/\partial\theta^4, \\ &= \textstyle\sum_n (n^2-n^4)a_n(\beta). \end{aligned} \qquad (10)$$

If Eq. (9) is correct, $G(\beta)$ should scale in the continuum limit.

Numerically, $G(\beta)$ is hard to measure because it is the difference of two quantities, both of which are small for large β. We had to generate on the order of half a million configurations in order to compute $G(\beta)$ with reasonable accuracy in the region $\beta\geq 1.3$ where continuum behavior is expected.[1,3,7] The lattices we used in our simulations ranged in size from 10^2 to 25^2. Our results for $G(\beta)$ are given in Fig. 1. We also plot

$$\chi(\beta)=\langle Q^2\rangle/V$$

and

$$\chi_4(\beta)=\langle Q^4\rangle_c/V=(\langle Q^4\rangle-3\langle Q^2\rangle^2)/V$$

for comparison. Note that only $G(\beta)$ has the correct dependence on β required for it to have a meaningful continuum limit. Neither χ nor χ_4 scales correctly by itself. This is a good check of Eq. (9).

To study the free energy as a function of θ, we followed the method of Ref. 6. The system was

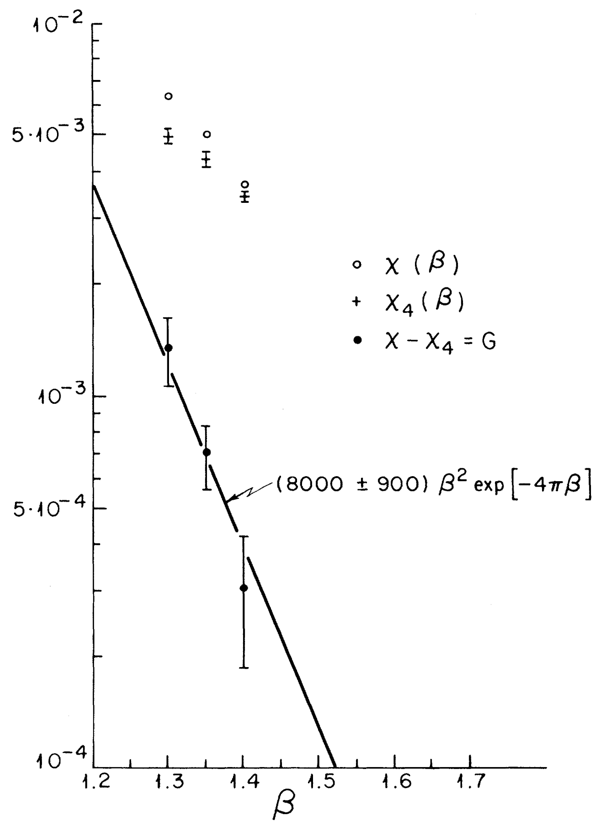

FIG. 1. $G(\beta)$ [see Eq. (10)] vs β from simulations on a 20^2 lattice. For comparison, $\chi(\beta)$ and $\chi_4(\beta)$ are also plotted. Note that only $G(\beta)$ scales correctly.

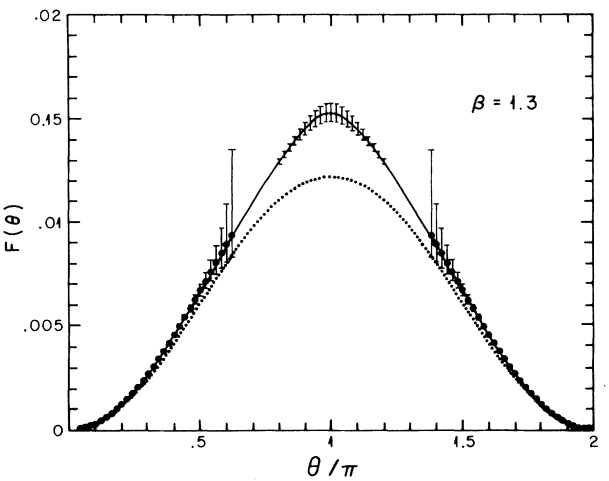

FIG. 2. The free energy F as a function of θ on lattices of size 15^2 (dotted line), 20^2 (solid line), and 25^2 (solid dots). The error bars on the 15^2 data are too small to plot. Those for the 20^2 lattice are only shown in the region near $\theta \approx \pi$. Away from this region, they are negligible. The 25^2 data and its associated error bars are only drawn for $\theta < 0.62\pi$ and for $\theta > 1.38\pi$. For θ in the central region near π, the 25^2 data were not accurate enough to plot.

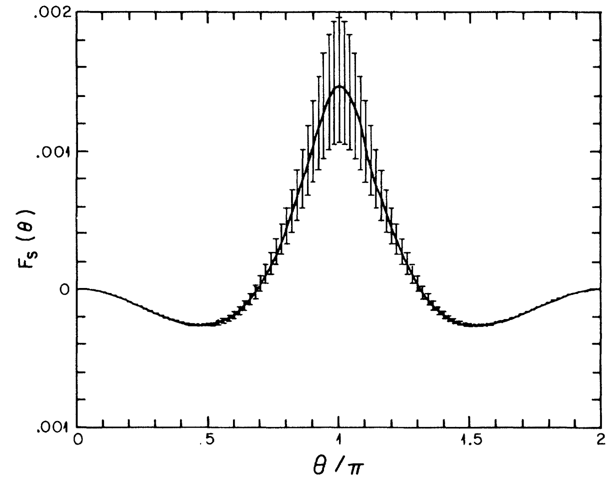

FIG. 3. The subtracted free energy $F_s(\theta) = F(\theta) - a_1(\beta)(1-\cos\theta)$ as a function of θ on a 20^2 lattice at $\beta = 1.3$.

simulated at $\theta = 0$ and a large set of thermalized configurations were generated. The topological charge distribution $P(Q)$ was computed from this set of configurations [$P(Q)$ is the fraction of configurations with charge Q]. The expectation value of an operator O is then approximated by,

$$\langle O \rangle = \langle O e^{i\theta Q} \rangle_{\theta=0} / \langle e^{i\theta Q} \rangle_{\theta=0}, \qquad (11)$$

where $\langle \ldots \rangle_{\theta=0}$ means expectations in the $\theta = 0$ ensemble. The free energy per unit volume is

$$F(\theta,\beta) = V^{-1} \ln \sum_Q P(Q) e^{i\theta Q}. \qquad (12)$$

The values of β we worked at were in the region from $\beta = 1.3$ to 1.5. The reasons we are forced to small values of β have already been explained elsewhere.[6] However, our β values are in the region where one expects scaling behavior to start appearing.[1,11] In Fig. 2 we plot the free energy F versus θ for $\beta = 1.3$. No phase transition occurs up to $\theta \approx 0.8\pi$. The appealing possibility of a phase transition at $\theta = \pi$ is still open. The data on lattices of size 20^2 and 25^2 agree with each other up to $\theta \approx 0.6\pi$ where the errors on the 25^2 lattice become large. This is evidence that these lattice sizes are sufficient ($\xi \leq 10$) for this range of β, θ. However, the results for F on the 15^2 lattice agree with the other curves up to $\theta \approx 0.2\pi$, but deviate from the other two lattice sizes for larger values of θ, clearly indicating that the correlation length is growing with θ for fixed β. Similar results were also obtained for the four-dimensional gauge theory.[6]

Finally, we define the subtracted free energy as follows:

$$F_s(\theta, \beta = 1.3) = F(\theta, \beta = 1.3) - a_1(1 - \cos\theta). \qquad (13)$$

For $\beta = 1.3$ the coefficient $a_1 = 0.0069$ is determined by a fit to the 20^2 data and F_s is plotted in Fig. 3. If a_1 were known exactly, this curve would be unchanged in the continuum limit, apart from a scale given by the renormalization group. Since a_1 is obtained from a fit, this is not strictly true for Fig. 3. However, the general shape of the curve is probably significant.

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