New Proposal for Numerical Simulations of θ-Vacuum-like Systems

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We propose a new approach to perform numerical simulations of θ-vacuum-like systems, test it in two analytically solvable models, and apply it to CP^3. The main new ingredient in our approach is the method used to compute the probability distribution function of the topological charge at $\theta = 0$. We do not get unphysical phase transitions (flattening behavior of the free energy density) and reproduce the exact analytical results for the order parameter in the whole θ range within a few percent.

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Quantum field theories with a topological term in the action have been a subject of interest in high energy particle physics and in solid state physics for a long time. In particle physics, these models describe particle interactions with a CP violating term. The extremely small experimental bound for the CP violating effects in QCD (strong CP problem) is still waiting for a convincing theoretical explanation [1]. In solid state physics, chains of half-integer quantum spins with antiferromagnetic interactions are related to the two-dimensional $O(3)$ nonlinear sigma model with a topological term at $\theta = \pi$. It has been argued that this model presents a second order phase transition at $\theta = \pi$, keeping its ground state CP symmetric (Haldane conjecture) [2].

Nonperturbative studies of field theories with a θ-vacuum term are enormously delayed because of the complex character of the Euclidean action which forbids the application of all standard Monte Carlo algorithms. Besides this, lattice QCD lacks from a simple consistent definition of topological charge.

The partition function $\mathcal{Z}_V(\theta)$ of any θ-vacuum-like model in a finite space-time lattice volume V can be written, up to a normalization constant, as the discrete Fourier transform of the probability distribution function (PDF) of the topological charge at $\theta = 0$:

$$\mathcal{Z}_V(\theta) = \sum_n p_V(n) e^{i\theta n}, \tag{1}$$

where $p_V(n)$ is the probability of the topological sector n and the sum runs over all integers n. In almost all practical cases the sum in (1) has a number of terms of order V since the maximum value of the topological charge at finite volume is of this order.

Since efficient algorithms for numerical simulations of physical systems with complex actions are not yet available, the only *a priori* reliable numerical scheme to analyze the thermodynamics of θ-vacuum-like models goes through the determination of the PDF of the topological charge, $p_V(n)$, and the evaluation of its Fourier transform (1). But this is a difficult task due to the following two technical reasons, which will be clarified later: (i) any numerical determination of $p_V(n)$ suffers from statistical fluctuations [3], and small errors in $p_V(n)$ can induce enormous relative errors in the determination of a quantity as $\mathcal{Z}_V(\theta)$ which is an extremely small number of order e^{-V}, (ii) even if we were able to evaluate pV(n) with infinite precision, the sum in (1) contains terms that differ by many orders of magnitude, running from 1 to e^{-V} [4].

In a few specific cases one can overcome the sign problem [5]. However, previous attempts by other groups to simulate θ-vacuum-like systems [3,6] were based on the numerical determination of the PDF of the topological charge straightforwardly, by standard simulations, or by more sophisticated methods based on the use of multibinning and reweighting techniques. In all these attempts, artificial phase transitions at a θ_c decreasing with the lattice volume were observed for the two-dimensional U(1) gauge theory at strong coupling as well as CP^N models. The origin of this artificial behavior, which follows from a flattening behavior of the free energy for θ values larger than a certain θ_c, was analyzed in [3,7]. Both groups agreed that the observed behavior was produced by the small statistical errors in the determination of the PDF of the topological charge, the effect of which became more and more relevant as the lattice volume was increased. In Ref. [7] it was also noticed that by smoothing the PDF flattening disappears.

The purpose of this Letter is to introduce a new numerical approach to simulate θ-vacuum-like models. This approach is based on a new method to compute the PDF of the topological charge and the use of a multiprecision algorithm in order to compute the sum in (1) with a precision as high as desired.

For reasons which become apparent in what follows, let us write the partition function (1) as a sum over the density of topological charge $x_n = n/V$ and set $p_V(n) = \exp[-V f_V(x_n)]$, where $f_V(x)$ is a smooth interpolation of $-1/V \ln p_V(x_n)$:

$$\mathcal{Z}_V(\theta) = \sum_{x_n} e^{-V f_V(x_n)} e^{i\theta V x_n}. \tag{2}$$

Equation (2) defines a 2π periodic function of θ. Since CP is a symmetry of the action at $\theta = 0$ and $\theta = \pi$, $f_V(x)$ will be an even function. We will assume that CP is realized in the vacuum at $\theta = 0$ since otherwise the theory would be ill-defined at $\theta \neq 0$ [8]. This implies that $\exp[-Vf_V(x_n)]$ will approach a delta distribution centered at the origin in the infinite volume limit. In some exceptional cases, as QCD in the chiral limit, the function $f_V(x)$ is not defined since any topological sector with nonvanishing charge has a vanishing probability. However, this is a trivial case in which the theory is independent of θ.

Let us consider the partition function (2) in the complex θ plane, in particular, on the imaginary axis $\theta = -ih$, and let $f(x)$ be the infinite volume limit of $f_V(x_n)$. All the terms entering Eq. (2) are positive definite, and then in the infinite volume limit the free energy is given by the saddle point. Assuming that $f(x)$ has first derivative for any x except at most in isolated points, we can write the saddle point equation:

$$f'(x) = h, \tag{3}$$

which gives the external "magnetic field" h as a function of the density of topological charge x.

Our proposal to compute the function $f(x)$ is based on the following three steps:

(i) To perform standard numerical simulations of our system at imaginary $\theta = -ih$ and to measure the mean value of the density of topological charge as a function of h with high accuracy (typically a fraction of a percent). This is feasible since the system we have to simulate has a real action. Then, Eq. (3) is used to get a numerical evaluation of $f'(x)$.

(ii) To get $f(x)$ we have to integrate $f'(x)$. Of all the possible ways to do this integral, we decided to fit $f'(x)$ by the ratio of two polynomials, whose order is chosen to obtain a high quality fit, and then to perform analytically the integral of the fitting function. In this way we get a very precise determination of $f(x)$, which allows us to compute the PDF in a range varying several thousands of orders of magnitude. This is the main advantage of our approach when compared with other methods based on a direct computation of $p_V(n)$.

(iii) To use a multiprecision algorithm to compute the partition function (2) using as input the function $f(x)$ previously determined.

The function $f(x)$ obtained in step (ii) suffers from statistical and systematic errors, the last coming from the fact that the saddle point Eq. (3) has finite volume corrections. An analysis of these errors for the models and sizes we have studied (see below) shows that systematic errors due to finite volume effects are smaller than the statistical ones in the whole relevant range of x. This is the reason why we will replace $f_V(x_n)$ in Eq. (2) by its asymptotic value $f(x_n)$ in what follows. This substitution has no effect in the infinite volume limit at imaginary θ and we are assuming that the same holds for real θ.

Before presenting our results for the various testing models we have analyzed, let us briefly discuss how errors in the determination of $f(x)$ can propagate to $\mathcal{Z}_V(\theta)$. This is an important point since, as pointed out in [3,7], the artificial phase transitions found in U(1) and CP^N were caused by the statistical errors in the determination of the PDF.

To this end, let $f_V(x_n)$ be the exact value at a given lattice volume V of the function which parametrizes the PDF and be $\Delta f_V(x_n)$ a given deviation from the exact value. If we denote by $\mathcal{Z}'_V(\theta)$ the partition function computed with $f_V(x_n) + \Delta f_V(x_n)$, a simple calculation tells us that this partition function is related with the exact partition function $\mathcal{Z}_V(\theta)$ as follows:

$$\mathcal{Z}'_V(\theta) = \mathcal{Z}_V(\theta)\langle e^{-V\Delta f_V(x_n)}\rangle. \tag{4}$$

We can at this point analyze two extreme cases. First let us assume that $\Delta f_V(x_n)$ vanishes everywhere except at a given x_m. Taking into account that the partition function $\mathcal{Z}_V(\theta)$ which enters in the denominator of the expectation value $\langle e^{-V\Delta f_V(x_n)}\rangle$ should behave as $e^{-Vg_V(\theta)}$, where $g_V(\theta)$ is the free energy density [$g_V(0) = 0$], we should get

$$\langle e^{-V\Delta f_V(x_n)}\rangle = 1 + 2e^{-V[f_V(\frac{m}{V}) - g_V(\theta)]}(e^{-V\Delta f_V(\frac{m}{V})} - 1)\cos(m\theta). \tag{5}$$

Since $g_V(\theta)$ is an increasing function of θ, it will be smaller than $f_V(x_m)$ near the origin, and therefore the free energy density computed with the modified partition function will differ from the exact one of a small quantity of order $\frac{1}{V}$ in this region. However, at larger values of θ the function $g_V(\theta)$ can become larger than $f_V(x_m)$ and in such a case the correction to the free energy density will be finite or, even worse, the modified partition function can become negative. The other extreme case is that in which we assume that the error $\Delta f_V(x_n)$ is constant. Under such an assumption Eq. (4) implies that the error in the free energy density $g_V(\theta)$ will also be Δf_V.

The previous discussion, as the results of [7], suggests that correlated errors propagate in a less dramatic way than uncorrelated ones, and this would be a good scenario for numerical methods which, as in our approach, produce correlated errors in the determination of $f_V(x_n)$. We have checked this interesting issue in the two-dimensional U(1) model at strong coupling (see below) and verified that, in fact, correlated errors in $f_V(x_n)$ induce errors of the same order in the free energy density $g_V(\theta)$.

To test these ideas we have analyzed three models: the one-dimensional antiferromagnetic Ising model within an external imaginary magnetic field, the two-dimensional compact U(1) model with topological charge, and CP^3 in two dimensions. The coupling to the imaginary magnetic field in the Ising model can be

written as $i\theta k_B T/2\sum_i S_i$, where k_B is the Boltzmann constant and T is the temperature. For an even number of spins, the quantity $1/2\sum_i S_i$ is an integer taking all values between $-N/2$ and $N/2$, and therefore it can be seen as a quantized charge. Furthermore, the theory has a Z_2 symmetry at $\theta = 0$ and $\theta = \pi$ which is analogous of CP in field theory. We use the notation $F = J/k_B T$, where J is the coupling constant between nearest neighbors. The transfer matrix technique allows one to solve analytically the model. For antiferromagnetic couplings, $F < 0$, the magnetization is an analytic function of θ between $-\pi$ and π. At $\theta = \pi$ the system shows a first order phase transition with a nonvanishing magnetization. From a numerical point of view the determination of the free energy density and order parameter through Eq. (1) in this model has the same level of complexity of more sophisticated models. Furthermore, in contrast to two-dimensional U(1) gauge theory, where the PDF of the topological charge is nearly Gaussian, the non-Gaussian behavior of the PDF of the mean magnetization in the antiferromagnetic Ising model makes this model a good laboratory to check the reliability of our approach. Figure 1 shows our numerical results for the order parameter versus θ for a linear chain of 1000 spins and $F = -1/2$. Statistical errors were estimated by doing ten samples of the numerical results and applying a jackknife analysis. The PDF of the order parameter for such a system takes values in a range of around 2000 orders of magnitude. Notwithstanding that, we are able to reproduce the order parameter in the whole θ interval within a few percent.

The two-dimensional compact U(1) gauge model with the θ angle at strong coupling constitutes another interesting check because we can compare the goodness of our approach with the other existing simulations which showed artificial behavior with a fictitious phase transition moving to the origin when increasing the lattice volume. Figure 2 displays our results for the topological charge density versus θ in a 80×80 lattice at $\beta = 0$ and $\beta = 0.6$. We are able to reproduce the exact result within a few per thousand in the whole θ interval. The agreement between analytical and numerical results is actually impressive. Furthermore, the flattening found in [3] for the free energy density in relatively small lattices is absent in our simulations even in the 80×80 lattice.

To test how different kinds of errors in the determination of the function $f(x)$ which defines the PDF of the density of topological charge can affect the determination of the free energy and order parameter, we have added to the measured $f(x)$ a random relative error of order 10^{-3}. Figure 3 shows the order parameter obtained in this way. As can be seen a small but random error in $f(x)$ propagates to the order parameter in a very dramatic way and makes the calculation meaningless. Contrary to that if, in order to simulate a correlated relative error of order up to 50%, we replace the measured $f(x)$ by the (even) function $f(x)(1 + 0.5\sin(x^2))$, the result for the order parameter is practically indistinguishable from the exact value for $\theta < \pi/2$, and the maximum deviation is about 25%, at $\theta = \pi$ (see Fig. 3). We conclude that random errors in $f(x)$ propagate in a very dramatic way but correlated errors do not, and this helps one to understand why our approach works so well.

The last model we have analyzed is CP^3 in two-dimensional Euclidean space. It is the standard wisdom that this model shares many qualitative features with QCD. Even if it has not been analytically solved we believe it is worthwhile to compare our results with previous existing numerical simulations. We studied the lattice formulation that makes use of an auxiliary U(1) field. Also in this model, the previous numerical simulations gave artificial phase transitions with a flattening

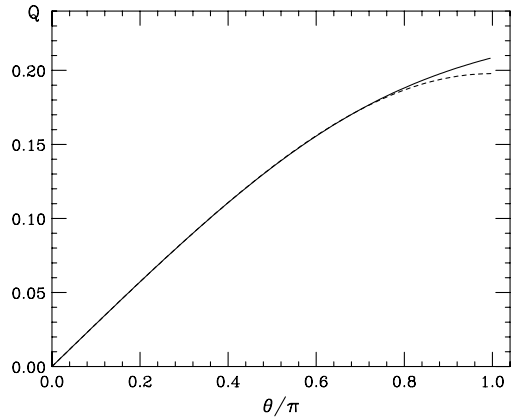

FIG. 1. Magnetization versus the imaginary magnetic field in the one-dimensional antiferromagnetic Ising model at $F = -1/2$ on a chain of 1000 sites: exact (dashed curve) and numerical (continuous curve) results. Statistical errors are smaller than 2%.

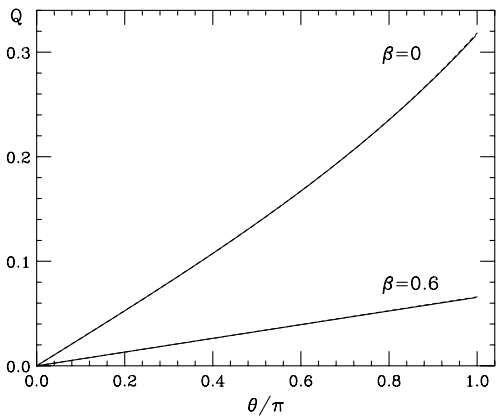

FIG. 2. Topological charge versus θ in the two-dimensional U(1) model at $\beta = 0$ and $\beta = 0.6$ on a 80×80 lattice. Statistical errors are not visible at this scale. The exact result (dashed curve) cannot be distinguished from the numerical result (continuous curve).

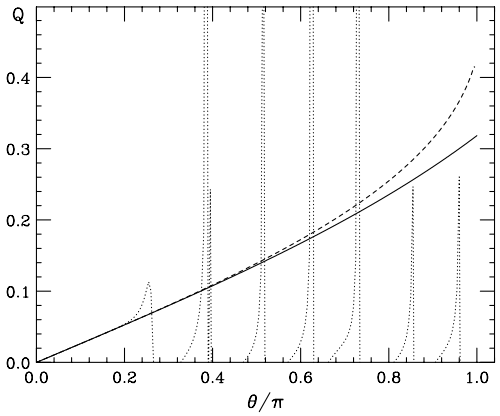

FIG. 3. Topological charge versus θ in the two-dimensional U(1) model at $\beta = 0$. The continuous curve is the exact result, the dashed curve is the result obtained by substituting $f(x)$ by $f[x](1 + \frac{1}{2}\sin(x^2))$, and the dotted curve is the result obtained by adding a random error of the order of 0.1% to $f(x)$.

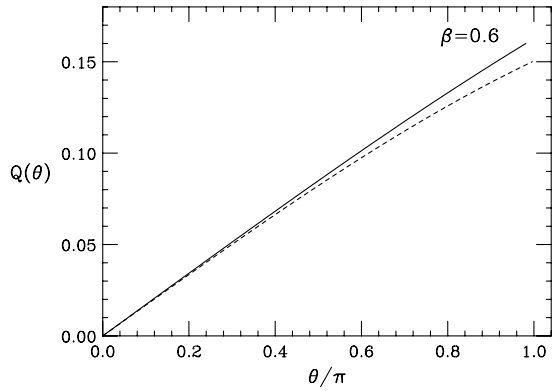

FIG. 4. Topological charge versus θ in the two-dimensional CP^3 model at $\beta = 0.6$ on a 100×100 lattice. The continuous line (discontinuous line) reports the results obtained fitting $f'(x)$ with a polynomial (the ratio of two polynomials). Statistical errors are at the 1% level.

behavior for the free energy density at a θ_c decreasing with the lattice volume [3,6].

Figure 4 shows our results for the order parameter versus θ at $\beta = 0.6$ on a 100^2 lattice. We have chosen this particular β value in order to compare directly with results reported in [3]. In our simulations we have no trace of the fictitious phase transition found in [3]. Furthermore, the order parameter is clearly different from zero at $\theta = \pi$; hence CP is spontaneously broken at this β value. An open question is how CP is realized in the continuum limit [9]. A more extensive analysis of this model, including a study of the behavior of the order parameter in the continuum limit, and an analysis of statistical and systematic errors involved in our approach, will be published elsewhere. What is interesting to notice here is that our results do not suffer from artificial phase transitions caused by statistical errors in the determination of the PDF.

In the three models analyzed the finite size effects in $f'(x)$ cannot be appreciated since they are completely masked by the small statistical errors. For instance, finite size effects can be exactly computed in the Ising model: they are exponentially small with the lattice size. This is a general feature of noncritical systems. However, volume effects might be troublesome in the analysis of the continuum limit. Concerning systematic errors due to the choice of a particular fitting function for $f'(x)$, the difference between the numerical and exact results for the Ising and compact U(1) models (beside the statistical errors) reported in Figs. 1 and 2 give us an idea of the order of magnitude of these errors. Of course systematic errors can depend on the model as well as on the parameters. In CP^3 at $\beta = 0.6$ we did also a five-parameter polynomial fit of the data for $f'(x)$ in the relevant x interval. The discrepancy between the topological charge density obtained in the two cases is at most 7% (see Fig. 4).

Similar ideas to those presented in this work have been proposed and promisingly applied to a matrix model of QCD at finite density in [10].

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