θ-Vacuum Systems Via Real Action Simulations

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ABSTRACT

Inspired by the results of the Ising model within an imaginary external magnetic field, we introduce a transformation in quantum systems with a θ-vacuum term that amounts to a rescaling of $z = \cos(\frac{\theta}{2})$. Making use of this transformation we are able to determine the order parameter as a function of θ. The approach is successfully tested in models with both broken and unbroken $CP$ symmetry at $\theta = \pi$. 
Quantum systems with complex euclidean actions have received an important amount of attention in recent time. Indeed there are two very relevant subjects in quantum field theory the analysis of which requires the use of complex actions: the study of topological structures and the behavior of matter at high temperature and density. Notwithstanding the big interest in these subjects, it is currently not possible to write an efficient code to perform numerical simulations of systems with complex actions. All efficient algorithms to simulate statistical systems are based in the use of a true probability distribution function as Boltzmann weight. This is the reason why all attempts to analyze systems with complex actions are based (i) on the use of specific properties of the particular model under study [1], (ii) uncontrolled analytical continuations, or (iii) in a very delicate process of summing up all the contributions which appear in the definition of the partition function [2], [3], [4], [5], [6].

In a recent paper [7] we proposed a new approach to analyze systems with a $\theta$-vacuum term, tested it in two analytically solvable models, and applied to the study of $\text{CP}^3$ with a topological term in the strong coupling region. This approach is based on the use of a high accuracy method to measure the probability distribution function of the topological charge density at $\theta = 0$ from numerical simulations at imaginary $\theta$. It is combined with a multiprecision algorithm which allows to sum up all the terms which appear in the partition function, that differ by many orders of magnitude, running from 1 to $e^{-V}$, where $V$ is the lattice volume.

Even if the results reported in [7] are quite promising, the method is not free from systematics and it would be therefore important to have alternative approaches available in order to compare physical predictions. This is indeed the purpose of present paper.

We should say from the beginning that contrary to the approach reported in [4] where no assumption on the phase structure of the system was made, here we will make the assumption that the system has no phase transition at real $\theta$ except at most at $\theta = \pi$. This means that our proposal should be used in practice as complementary to other approaches and one should look for consistency between their results.

The method is based in extrapolating a suitably defined function to the origin. The function turns out to be very smooth in all the cases we have considered up to now and this makes us confident on the whole procedure. At the very end it is equivalent to an analytical continuation from imaginary to real $\theta$. However it has not to be confused with analytical continuation of the free energy density and/or the order parameter which are extremely sensitive
to statistical errors and to the choice of fitting functions and therefore with small or no practical utility.

To fix the ideas and to keep this paper selfcontained, let us write the general form of the partition function of a system with a topological $\theta$-term as a sum over all topological sectors of the partition functions for each sector weighted with the proper topological weight,

$$Z_V(\theta) = \sum_n p_V(n) e^{i\theta n},$$  \hspace{1cm} (1)

where $p_V(n)$ is, up to a normalization constant, the probability of the topological sector $n$ at $\theta = 0$, and the sum runs over all integers $n$. Writing equation (1) one needs to assume that $CP$ symmetry is realized at $\theta = 0$ since otherwise $Z_V(\theta)$ would be ill-defined [8].

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. The partition function (1) can also be written as a sum over the density of topological charge $x_n = n/V$, and setting $p_V(n) = \exp[-V f_V(x_n)]$ one gets:

$$Z_V(\theta) = \sum_{x_n} e^{-V f_V(x_n)} e^{i\theta V x_n}. \hspace{1cm} (2)$$

Equation (2) defines a $2\pi$ periodic function of $\theta$. For models $CP$-invariant at $\theta = 0$ $f_V(x_n)$ is an even function; this property allow us to write:

$$Z_V(\theta) = \sum_{y_n} G_V(y_n) \left( \cos^2 \frac{\theta}{2} \right)^{V y_n} \hspace{1cm} (3)$$

where $y_n$, which is non negative by construction, takes the same non negative values as $x_n$ and $G_V(y_n)$ is a functional of $f_V(x_n)$. The mean value $y(\cos \frac{\theta}{2})$ of $y_n$ computed from (3) is related to the mean value $x(\theta)$ of $i$ times the density of topological charge as follows:

$$x(\theta) = i y \left( \cos \frac{\theta}{2} \right) \tan \frac{\theta}{2} \hspace{1cm} (4)$$

which shows explicitly the $2\pi$ periodicity. At imaginary $\theta$, $\theta = -i\hbar$, the previous equation becomes

$$x(-i\hbar) = y \left( \cosh \frac{\hbar}{2} \right) \tanh \frac{\hbar}{2} \hspace{1cm} (5)$$
Furthermore, at real \( h \), the system described by (1) can easily be simulated by standard numerical algorithms since in this case the Boltzmann weight is well defined. From numerical simulations at real \( h \) one can get \( y(z) \) for values of the argument \( z = \cosh \frac{h}{2} \) between 1 and \( \infty \). In order to get the topological charge density at real \( \theta \) one should extend this function to the \((0,1)\) interval in \( z \). But as stated before, an extension of \( y(z) \) is sensitive to statistical errors and fitting functions so that it makes this procedure not reliable.

The function \( y(z) \) depends also on the couplings of the model under consideration. For the one-dimensional Ising model within an external real or imaginary magnetic field \( h \), the function \( y(z) \) can be analytically computed and the final result is

\[
y(z) = \frac{(e^{-4F} - 1)^{-1/2} z}{(1 + (e^{-4F} - 1)^{-1} z^2)^{1/2}}\tag{6}
\]

which shows explicitly how this model, at imaginary values of the magnetic field \((0 < z < 1)\) and antiferromagnetic couplings \((F = \frac{j}{kT} < 0)\) breaks spontaneously the \(Z(2)\) symmetry at \( h = i\pi \) (see (4)). But this model shows also a very interesting property: a change in the coupling \( F \), or what is the same, a change in the physical temperature \( T \), is equivalent to a rescaling of the variable \( z \) since \( y \) depends on \( z \) through the combination \( e^{\lambda} z \), with \( \lambda = -\log(e^{-4F} - 1) \). In other words, if we define the transformation:

\[
y_\lambda(z) = y\left(e^{\frac{\lambda}{2}} z\right)\tag{7}
\]

which would allow us, for negative values of \( \lambda \), to extend the order parameter from imaginary \( \theta \) to real \( \theta \), the \( 1-d \) Ising model shows the exceptional feature that the transformation (7) is equivalent to a change of the coupling. This property, if true for other models, would be extremely interesting since it would reduce the problem of complex actions to simulations with real actions. Unfortunately this seems not to be the case since it is easy to check that already compact \( U(1) \) in two dimensions with a \( \theta \)-term does not exhibit such a property. However this is not the end of the story and we will try in what follows to make use of transformation (7) in a much less ambitious way.

Many of the physically relevant models, as \( \text{CP}^{N-1} \) or \( \text{QCD} \), are asymptotically free. Asymptotic freedom implies that the continuum limit is reached in the weak coupling region, but in this region the order parameter (and \( y(z) \)) will be very small for values of \( z \) near 1 since the density of topological structures in lattice units is very suppressed at weak coupling. This means
that, from simulations at real \( h \), we can plot \( y_\lambda/y \) against \( y \) up to values of \( y \) very close to the origin, provided that \( y(z) \) does not vanish for \( z > 0 \). We cannot exclude this possibility completely, but it does not happen in any of the exactly solvable models we know. Indeed, it is easy to show that \( y(z) \neq 0 \) for \( z > 0 \) if all the coefficients \( G_V(y_n) \) entering the right hand side of equation (8) are positive, as it happens in the models studied in the present work. In such a case, the fluctuation-dissipation theorem ensures that \( y(z) \) is a non decreasing function of \( z \). Furthermore, if the order parameter does not diverge at \( \theta = \pi \), \( y(z) \) should vanish at least linearly with \( z \) at \( z = 0 \) (that corresponds to \( \theta = \pi \)).

Moreover, if \( y_\lambda/y \) as a function of \( y \) shows a smooth behavior near \( y = 0 \), we can expect a simple extrapolation to \( y = 0 \) being reliable. This point is crucial in what follows and obviously can not be taken for granted. Apart from being reasonable it has been verified in all the models whose analytical solution is known to us. In particular it is true for the one-dimensional Ising model, compact \( U(1) \) in two dimensions, \( \text{CP}^3 \), and a toy model that exhibits no phase transition at \( \theta = \pi \), thus covering all the possible different qualitative possibilities.

In the Ising case we have done simulations of the model within an external real magnetic field \( h \) at \( F = -2.0 \). This coupling was chosen in order to be in the "weak coupling region" where \( y(z) \) is small near \( z = 1 \). The model breaks spontaneously the \( Z(2) \) symmetry at \( \theta = -ih = \pi \) and therefore \( y(z) \) vanishes linearly with \( z \) (see (4), (5)).

If we define an effective exponent \( \gamma_\lambda \) by the following equation:

\[
\gamma_\lambda = 2 \lambda \log \left( \frac{y_\lambda}{y} \right)
\] (8)

this exponent, in the limit \( y(z) \to 0 \) (\( z \to 0 \)), will give the dominant power of \( y(z) \) as a function of \( z \) near \( z = 0 \). A value for this exponent that goes to 1 when \( y \to 0 \) will imply spontaneous symmetry breaking, and values between 1 and 2 will signal a second order phase transition at \( \theta = \pi \) with a divergent susceptibility. The reason is that the order parameter, \( x = \tan(\theta/2)y[\cos(\theta/2)] \), will behave as \( (\pi - \theta)^{\gamma_\lambda - 1} \) for \( \theta \to \pi \).

Fig. 1 reports \( y_\lambda/y \) against \( y \) for the Ising model at \( \lambda = 0.5 \). The solid line is a quadratic fit of the points. This figure contains also the results for the effective exponent \( \gamma_\lambda \) against \( y \) (lower points). A simple quadratic fit predicts \( \gamma_\lambda(0) = 0.997(3) \) i.e., spontaneous symmetry breaking. We have checked that, as expected, we get compatible results using different values of \( \lambda = O(1) \), and the same is true for the rest of the models considered.
The fit of $y_{\lambda}/y$ against $y$ together with the dependence of $y(z)$ on $z$ for $z \geq 1$ (computed from numerical simulations at real $h$) allows one to reconstruct the order parameter $\Pi$ at real $\theta$. To simplify the discussion let us assume we have computed $y(z_0) = y^0$. Next using the fit of Fig. 1 we plot $y_{\lambda}$ against $y$ and look in this plot for the value of $y = y^1$ which corresponds to $y_{\lambda} = y^0$ (see Fig. 2). It is simple to verify that $y^1 = y(e^{-\lambda/2}z_0)$. The next step is to iterate this procedure: we replace $y^0$ by $y^1$ and get $y^2 = y(e^{-\lambda}z_0)$, and so on. Once we have computed in this way $y(z)$ for as many values of $z \leq 1$ as desired, the order parameter can be computed using equation $\Pi$.

Fig. 3 contains the results for the Ising order parameter. We report also in this figure the exact analytical results in order to put in evidence the agreement.

For two-dimensional compact $U(1)$ with topological charge we chose to work at $\beta = 1.0$ and $\lambda = 0.5$. Figures similar to 1 and 3 were obtained for this model. The agreement between numerical and analytical results for the order parameter was even better than for the Ising model. Because of space limitations the corresponding figures are not included.

The next model we want to analyze here is CP$^3$ with topological charge. Contrary to the Ising and two-dimensional compact $U(1)$ cases, in which we can compare with the exact analytical results, CP$^N-1$ models, which share many interesting properties with $SU(N)$, are not analytically solvable.

We have adopted for the action the “auxiliary $U(1)$ field” formulation:

$$S_g = N\beta \sum_{n,\mu} (\bar{z}_{n+\mu}z_nU_{n,\mu} + \bar{z}_n\bar{z}_{n+\mu}\bar{U}_{n,\mu} - 2)$$

(9)

where $z_n$ is a $N$-component complex scalar field that satisfies $\bar{z}_n z_n = 1$ and $U_{n,\mu}$ is a $U(1)$ “gauge field”. The topological charge operator can be constructed directly from the $U(1)$ field:

$$S_\theta = i\frac{\theta}{2\pi} \sum_p \log(U_p)$$

(10)

where $U_p$ is the product of the $U(1)$ field around the plaquette and $-\pi < \log(U_p) \leq \pi$.

Simulations were done at $\beta = 0.4$. This value of the coupling is not in the weak-coupling scaling region, but the values of $y(z)$ near $z = 1$ are smooth enough to allow a simple extension of $y_{\lambda}/y$ until $y = 0$. Fig. 4 contains the effective exponent $\gamma_{\lambda}$ against $y$ at $\lambda = 0.5$. A simple quadratic fit predicts $\gamma(0) = 1.03(5)$ i.e., spontaneous symmetry breaking at $\theta = \pi$. By imposing,
as suggested by the previous fit, $\gamma(0) = 1.0$ in the fit of $y_\lambda/y$ against $y$, we get for the order parameter the results reported in Fig. 5. The continuous line in this figure represents the numerical results obtained within the approach reported in [7]. The very good agreement between the two approaches makes quite reliable the numerical results and $CP$ structure at $\theta = \pi$ of Fig. 5.

The models previously analyzed have a common feature: $CP$ symmetry is always spontaneously broken at $\theta = \pi$. In order to check that our approach works also in the symmetric case we have analyzed a simple toy model, with only one effective degree of freedom, where $CP$ symmetry is enforced at $\theta = \pi$. This model, which resembles very much the free instanton gas model, is described at finite volume $V$ by the following partition function:

$$Z_V(\theta) = (1 + A \cos \theta)^V.$$  \hfill (11)

The order parameter at real $\theta$

$$x(\theta) = i \frac{A \sin \theta}{1 + A \cos \theta}$$  \hfill (12)

shows explicitly $CP$ symmetry at $\theta = \pi$, as it should be since this is a model of one degree of freedom. We have not done for obvious reasons numerical simulations of this model at real $h = -i\theta$ but in order to work in realistic conditions, we modified the exact value of the order parameter at real $h$ by adding to it a random gaussian error of 1 percent. Fig. 6 contains the exact analytical results for the order parameter at $A = 0.005$ and the points obtained within our approach, using always for the parameter $\lambda$ defined in [7] the value 0.5. The agreement is quite good.

A final comment on the possibility of applying this approach to the inverse problem i.e., finite density $QCD$, is worthwhile. $QCD$ at imaginary chemical potential and staggered fermions can be simulated numerically because the fermion determinant is positive definite. Its partition function belongs to the general class of partition functions described by [2], where $x_n$ now stands for the density of baryonic charge and $\exp[-V f_V(x_n)]$ is the probability distribution function of the baryon density at vanishing chemical potential. From numerical simulation of $QCD$ at imaginary chemical potential one can measure the mean value of the density of baryonic charge and from it we can get $y(z)$ for $z$-values between 0 and 1. In order to get the density of baryonic charge at real chemical potential we should extend $y(z)$ to $z$-values larger than 1. Summarizing we know $y_\lambda/y$ as a function of $y$ around $y = 0$ and we need to extend this quantity to larger values of $y$. But since a phase transition is expected in $QCD$ at finite chemical potential, a singular behavior of
$y_{\lambda}/y$ as function of $y$ should also be expected, and any analytical extension of this quantity should fail when trying to reproduce the correct behavior.

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Figure 1: $y_\lambda/y$ and $\gamma_\lambda$ as a function of $y$ for $\lambda = 0.5$ in the Ising model ($F = -2.0$).
Figure 2: An example of the iterative procedure to reconstruct $y(z)$: $y_\lambda$ as function of $y$ is plotted using dashed line in the region where direct measurements are available and continuous line in the extrapolated region. The straight continuous line is $y_\lambda = y$. 
Figure 3: The order parameter in the Ising model ($F = -2.0$). Continuous line is the exact result, points have been obtained from quadratic fit of $y \lambda / y$ data reported in Fig. 1.
Figure 4: CP$^3$ model at $\beta = 0.4$ in a 100x100 lattice: the effective exponent $\gamma_\lambda$ versus $y$. The continuous curve is a quadratic fit to the data.
Figure 5: $\text{CP}^3$ model at $\beta = 0.4$ in a 100x100 lattice. The order parameter as a function of $\theta$ from the fit of Fig. 4 (points) and the same quantity using the algorithm proposed in [8].
Figure 6: The CP symmetric model presented in the text: numerical (points) and exact (line) results.