

θ -Vacuum— Phase Transitions and/or Symmetry Breaking at $\theta = \pi$ —Vicente AZCOITI,¹ Angelo GALANTE^{2,3} and Victor LALIENA¹¹*Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain*²*Dipartimento di Fisica dell'Università di L'Aquila, 67100 L'Aquila, Italy*³*INFN, Laboratori Nazionali del Gran Sasso, 67010 Assergi, L'Aquila, Italy*

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Assuming that a quantum field theory with a θ -vacuum term in the action shows non-trivial θ -dependence and provided that some reasonable properties of the probability distribution function of the order parameter hold, we argue that the theory either breaks spontaneously CP at $\theta = \pi$ or shows a singular behavior at some critical θ_c between 0 and π . This result, which applies to any model with a pure imaginary contribution to the euclidean action consisting in a quantized charge coupled to a phase, as QCD, is illustrated with two simple examples; one of them intimately related to Witten's result on $SU(N)$ in the large N limit.

§1. Introduction

Quantum Field Theories with a topological term in the action are a subject of interest in high energy particle physics and in solid state physics since 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 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⁾

Non-perturbative studies of field theories with a θ -vacuum term are enormously delayed because of two technical reasons: first, there are difficulties in finding a consistent definition of topological charge for QCD in discrete space-time, preventing the use of the most powerful non-perturbative method, the lattice regularization; second, even in simpler QCD-like models, as CP^N or sigma models, for which a consistent definition of topological charge is known, the complex nature of the euclidean action forbids the application of all standard Monte-Carlo algorithms to perform numerical simulations (see for example Refs. 3) and 4)). We need therefore new ideas which, beside our present technical abilities, allow a progress in this field.

The θ -term breaks explicitly a Z_2 symmetry (CP), except at $\theta = 0$ and $\theta = \pi$. Most of the models the θ dependence of which is known break this symmetry spontaneously at $\theta = \pi$ (for an early study see Ref. 5)). An intriguing question in such a case is the realization of the 2π periodicity in θ .⁶⁾ For instance, in $SU(N)$

gauge theory at large N the θ dependence appears through the combination θ/N . The periodicity is realized by conjecturing that the vacuum energy density is a multi-branched function of the form

$$E(\theta) = N^2 \min_k H \left(\frac{\theta + 2\pi k}{N} \right). \quad (1.1)$$

This behavior occurs also in some two dimensional systems,^{7)–9)} and leads to spontaneous breaking of CP at $\theta = \pi$ in a natural way. Recently, Witten has shown that in $SU(N)$ gauge theories at large N Eq. (1.1) holds with $H(\theta) = C\theta^2$, where C is a positive constant independent of N .¹⁰⁾

We want to show in this paper that the above behavior is not specific of large N gauge theories but rather general. More precisely, we will argue that *any model with a quantized charge which is an order parameter of a given symmetry and which appears as an imaginary contribution to the euclidean action, either breaks the symmetry at $\theta = \pi$ or shows some singularity for θ -values between 0 and π , provided that there is a nontrivial θ -dependence.*

§2. General description

In the specific case of QCD, the partition function with a topological term in the action reads as follows:

$$\mathcal{Z} = \int [dA_\mu^a] [d\psi] [d\bar{\psi}] \exp \left\{ - \int d^4x [\mathcal{L}(x) - i\theta X(x)] \right\}, \quad (2.1)$$

where $\mathcal{L}(x)$ is the standard QCD Lagrangian and $X(x) = \frac{1}{16\pi^2} \epsilon_{\mu\nu\rho\sigma} \text{Tr} F_{\mu\nu} F_{\rho\sigma}(x)$ is the euclidean local density of topological charge, the normalization of which has been chosen in such a way that the topological charge, $\int d^4x X(x)$ be an integer. We will assume in what follows that the regularized theory preserves the quantization of the topological charge.

To start with the proof, let us write the partition function $Z_V(\theta)$ in a finite space-time volume, V , as a sum over all topological sectors, labeled by the integer n that gives the topological charge, of the partition functions of each sector, weighted with the proper topological phase:

$$Z_V(\theta) = \sum_n g_V(n) e^{i\theta n}, \quad (2.2)$$

where

$$g_V(n) = \int_n [dA_\mu^a] [d\psi] [d\bar{\psi}] \exp \left[- \int d^4x \mathcal{L}(x) \right] \quad (2.3)$$

is the standard partition function computed over the gauge sector with topological charge equal to n . The function $g_V(n)$ is, up to the normalization factor $\sum_n g_V(n)$, the probability $p_V(n)$ of the topological sector n at $\theta = 0$. If we define the mean

topological charge density as $x_n = n/V$, we can write the previous partition function as

$$\mathcal{Z}_V(\theta) = \sum_{x_n} h_V(x_n) e^{i\theta V x_n}, \quad (2.4)$$

where $h_V(x_n) = g_V(n)$ and the step Δx_n in the topological charge density is $1/V$.

We will try now to write the partition function $\mathcal{Z}_V(\theta)$ as a sum of “continuous” pseudo-partition functions, where the word continuous stands to indicate that the density of topological charge x entering the definition of this new pseudo-partition function will be a continuous variable. To this end, let the new $h_V(x)$ be any continuous smooth interpolation of $h_V(x_n)$ and let us define a new function of θ in the following way:

$$\mathcal{Z}_{c,V}(\theta) = \int dx h_V(x) e^{i\theta V x}. \quad (2.5)$$

Summing up the pseudo-partition functions $\mathcal{Z}_{c,V}(\theta + 2\pi m)$ for all integers m and using the following representation of the periodic delta function (Poisson summation formula):

$$\sum_m e^{i2\pi m V x} = \frac{1}{V} \sum_m \delta\left(x - \frac{m}{V}\right), \quad (2.6)$$

we get the following identity:

$$\mathcal{Z}_V(\theta) = V \sum_m \mathcal{Z}_{c,V}(\theta + 2\pi m), \quad (2.7)$$

which relates our QCD partition function $\mathcal{Z}_V(\theta)$ to the pseudo-partition functions $\mathcal{Z}_{c,V}(\theta + 2\pi m)$. Of course different interpolations of $h_V(x_n)$ will give different equivalent realizations of Eq. (2.7).

In deriving the above result we have assumed that the sum in m and the integral in x can be commuted. This is a working hypothesis on the properties of the $h_V(x_n)$ function and we will use it to derive some physical consequences. As will be evident in the next section, the validity of this assumption is confirmed in some examples where analytical calculations are possible. Notice also that the sum in (2.7) has nothing to do with the sum over different topological sectors. Each sector labeled by an integer m in (2.7) can get contributions from all topological sectors. If $\mathcal{Z}_{c,V}(\theta + 2\pi m)$ is positive for any integer m , the physical interpretation of these integer numbers is very simple. Indeed in such a case and in what concerns the infinite volume limit, the summation in (2.7) can be replaced by the maximum in m of $\mathcal{Z}_{c,V}(\theta + 2\pi m)$ (saddle point solution) and therefore the integers m will define metastable vacua which will decay to the true vacuum, the energy density of which is given by $\min_m \{-1/V \log \mathcal{Z}_{c,V}(\theta + 2\pi m)\}$ (see the first example discussed below).

The mean value of the density of topological charge can be written as

$$\langle x \rangle = \sum_m \langle x \rangle_{c,m} \frac{\mathcal{Z}_{c,V}(\theta + 2\pi m)}{\sum_n \mathcal{Z}_{c,V}(\theta + 2\pi n)}, \quad (2.8)$$

with

$$\langle x \rangle_{c,m} = \frac{\int dx x h_V(x) e^{i(\theta+2\pi m)Vx}}{\int dx h_V(x) e^{i(\theta+2\pi m)Vx}}. \quad (2.9)$$

Since x in Eqs. (2.5) and (2.9) is a continuous variable, the pseudo-partition function $Z_{c,V}(\theta)$ will not be a periodic function of θ and $\langle x \rangle_{c,m}$ needs not to vanish at $\theta = \pi$. The periodicity in θ of $Z_V(\theta)$ is however guaranteed because we must sum up $Z_{c,V}(\theta + 2\pi m)$ for all integer values of m . In the same way, CP is recovered as a symmetry of the action at $\theta = \pi$, because the $m = 0$ contribution to $\langle x \rangle$ in (2.8) is, at $\theta = \pi$, compensated by the $m = -1$ contribution, the $m = 1$ contribution compensates with $m = -2$ and so on. Therefore, the contributions of different sectors cancel each other, giving a vanishing density of topological charge at $\theta = \pi$. In the thermodynamic limit, however, one sector could dominate (see below) and this would imply that the limits $\theta \rightarrow \pi$ and $V \rightarrow \infty$ do not commute, giving rise to the spontaneous Z_2 breaking. We cannot exclude that $\langle x \rangle_{c,m}$ vanishes, by accident, for some integer m at $\theta = \pi$. Usually however it is assumed that if the mean value of a local operator vanishes, it is because some symmetry forces it to vanish. In our case, as previously discussed, the “action” in the pseudo-partition functions $Z_{c,V}(\theta + 2\pi m)$ is not CP invariant at $\theta = \pi$.

Equation (2.7) is valid for any value of θ . At $\theta = 0$ (or at imaginary values of θ) and in the infinite volume limit the sector $m = 0$ in (2.7) gives all the contribution to the partition function. This is a simple feature which follows from the fact that in this case all the terms in the summation (2.4) and the integrand in (2.5) are positive definite and then the partition functions (2.4) and (2.5) can be replaced, in the infinite volume limit, by the maximum of the summands and integrand respectively (saddle point solution). Since both maxima are coincident, we get the desired result.

Even if we cannot exclude on theoretical grounds a phase transition in QCD at $\theta = 0$, it seems not very likely. Then one expects that $m = 0$ sector dominates at least in some interval around $\theta = 0$. If this sector dominates for every θ between $-\pi$ and π , we will get a phase transition at $\theta = \pi$, with eventually a non-vanishing value of the topological charge density (remember the discussion following Eq. (2.9)) i.e. the theory will show spontaneous CP breaking. If by accident the density of topological charge computed in the $m = 0$ sector vanishes at $\theta = \pi$, we should get a continuous phase transition since in any case sector $m = -1$ will be the dominant one for θ values between π and 3π . The only way to avoid a phase transition at $\theta = \pi$ would be that the vacuum energy density of the $m = 0$ sector were a periodic function of θ with period equal to 2π . This, of course, is what happens in some trivial cases as QCD in the chiral limit, a limit in which there is no θ -dependence, or the dilute instanton gas approximation.¹¹⁾ The last case is a model of non-interacting degrees of freedom, the partition function of which factorizes as the product of V identical partition functions; and it is well known that phase transitions and critical phenomena are collective phenomena which appear as a consequence of the interaction of infinite degrees of freedom. Systems with non-interacting degrees of freedom are equivalent to systems with one degree of freedom and therefore they

cannot show phase transitions. Therefore we can say that, excluding trivial cases, periodicity of the $m = 0$ sector is not plausible.

The other possibility is that $m = 0$ sector dominates only until some critical θ_c less than π and then other sectors start to give a contribution to the partition function, in which case we will get a phase transition at this θ_c .

Since in the previous argumentation we have not made use of any specific property of QCD, except the quantization of the topological charge, our result applies to any model with a quantized charge which appears as an imaginary contribution to the euclidean action.

§3. Two simple examples

To see how this mechanism works in practical cases and to get intuition of what we can expect in physical systems, let us analyze in the following two simple examples: a model in which the probability distribution function of the density of topological charge at $\theta = 0$ is assumed to be gaussian and the Ising model within an imaginary external magnetic field.

The first example we want to discuss here includes models, as the quantum rotor,¹²⁾ with a density of topological charge at $\theta = 0$ distributed according to a gaussian distribution. Thus, let us assume that the function $h_V(x_n)$ which enters Eq. (2.4) has the form

$$h_V(x_n) = e^{-Vax_n^2}, \quad (3.1)$$

where a is a parameter related to the width of the distribution. This form of $h_V(x_n)$ is a natural assumption from a physical point of view as a first approximation to the actual distribution of nearly any model. In fact, outside second order phase transitions, the probability distribution function of intensive operators as the density of topological charge is expected to be gaussian in the vicinity of its maximum. Of course, deviations from the gaussian behavior far from the maximum can induce important changes in the θ -dependence of the theory in the large θ regime (as will become clear later). However, the gaussian distribution provides us with a simple model that can be analytically solved and gives useful insights on the general problem that we are addressing.

The partition function of the model is

$$\mathcal{Z}_V(\theta) = \sum_{x_n} e^{-Vax_n^2} e^{i\theta Vx_n}. \quad (3.2)$$

Even if this model can be solved without the help of Eq. (2.7), we will use it in order to clarify the relative weights of different sectors. The pseudo-partition function $\mathcal{Z}_{c,V}(\theta + 2\pi m)$ entering Eq. (2.7) can be analytically computed, and the final result is:

$$\mathcal{Z}_V(\theta) = \left(\frac{\pi V}{a}\right)^{1/2} \sum_m e^{-\frac{1}{4a}(\theta+2\pi m)^2 V}. \quad (3.3)$$

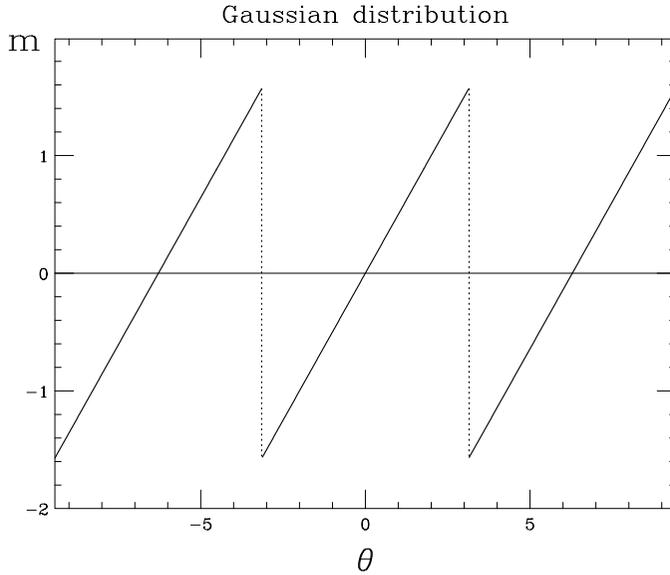


Fig. 1. Expectation value of the topological charge density as a function of θ in models with gaussian distribution.

If $|\theta| < \pi$, it is simple to verify that the free energy density $f(\theta)$ is given by $f(\theta) = \lim_{V \rightarrow \infty} \frac{1}{V} \log Z_V(\theta) = -\frac{1}{4a} \theta^2$. The $m = 0$ sector dominates for every θ between $-\pi$ and π . The vacuum expectation value of the density of topological charge, $\langle x \rangle$, is

$$\langle x \rangle = i \frac{\theta}{2a}, \quad |\theta| < \pi, \tag{3.4}$$

and the model breaks spontaneously parity at $\theta = \pi$ (see Fig. 1).

This simple case that, as we have seen, illustrates very well the results obtained in the first part of the paper, has also further relevance. In fact, using a duality relation of gauge theories with a large number of colors and string theory on a certain space-time manifold, Witten has recently studied the θ dependence of pure gauge theories in four dimensions¹⁰⁾ and found Eq. (3.4). The combination of both results strongly suggests that the probability distribution function of the topological charge density in pure $SU(N)$ gauge theory should be gaussian in the large N limit.

The second illustrative example is the one-dimensional Ising model within an imaginary external magnetic field. The hamiltonian of this model can be written as

$$H_N = -J \sum_{i=1}^N S_i S_{i+1} - i \frac{\theta k_B T}{2} \sum_{i=1}^N S_i, \tag{3.5}$$

where J is the coupling constant between nearest neighbors, k_B is the Boltzmann constant, T the physical temperature, N the number of spins, and we assume periodic boundary conditions. The partition function is given by

$$\mathcal{Z}_N = \sum_{\{S\}} e^{F \sum_i S_i S_{i+1} + i\theta \frac{1}{2} \sum_i S_i}, \quad (3.6)$$

where $F = J/k_B T$ and the sum is over all spin configurations.

For an even number of spins, the quantity $1/2 \sum_i S_i$ which appears in the imaginary part of the hamiltonian is an integer taking 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, in the spirit of this work, is the analogue of CP in QCD.

The transfer matrix technique allows to compute exactly the partition function defined in Eq. (3.6): $\mathcal{Z}_N = \lambda_+^N + \lambda_-^N$, where λ_{\pm} are the two eigenvalues of the transfer matrix

$$\lambda_{\pm}(\theta) = e^F \cos \frac{\theta}{2} \pm \left(-e^{2F} \sin^2 \frac{\theta}{2} + e^{-2F} \right)^{1/2} \quad (3.7)$$

and we get for the mean value of the density of magnetization

$$\langle x \rangle = i \frac{\sin(\theta/2)}{[e^{-4F} - \sin^2(\theta/2)]^{1/2}}, \quad |\theta| < \pi. \quad (3.8)$$

The solution for every θ between $-\pi$ and π is the analytical continuation of the solution for a real magnetic field.¹³⁾ Since in the real magnetic field case the $m = 0$ sector dominates always, this proves that the $m = 0$ sector dominates for every θ between $-\pi$ and π . A rather simple but long and straightforward calculation based on the analytical computation of the probability distribution function of the density of magnetization allows to demonstrate also this result, but the calculation is too long to be included here.

For θ -values between π and 3π ($-\pi$ and -3π) the $m = -1$ ($m = 1$) sector dominates (λ_- becomes larger than λ_+ in absolute value) and so on. Then we get, as expected, a periodic solution which shows a first order phase transition at $\theta = \pi$ with spontaneous Z_2 breaking (see Fig. 2).

In the ferromagnetic case ($F \geq 0$), the order parameter shows a divergence at a critical $\theta_c(T)$ running from 0 to π ^{14),16)} and the model is ill defined for $\theta_c(T) < \theta < \pi$.

§4. Discussion

Our main result, i.e., the existence of some singularity at θ_c between 0 and π , was conjectured for non-abelian gauge theories by 't Hooft¹⁷⁾ in 1981. Based on the applicability of Poisson summation formula, it is verified by the two simple examples previously discussed and also by other models with well established results as CP^N models in the strong coupling region,^{8),9)} two dimensional QED,⁷⁾ or high temperature QCD at imaginary chemical potential,^{18),19)} where the imaginary chemical potential plays the role of θ and the quantized charge is the baryonic charge. However it still seems to be in contradiction with some predictions of chiral effective models of QCD.^{20),21)} In these models the vacuum energy density is obtained,

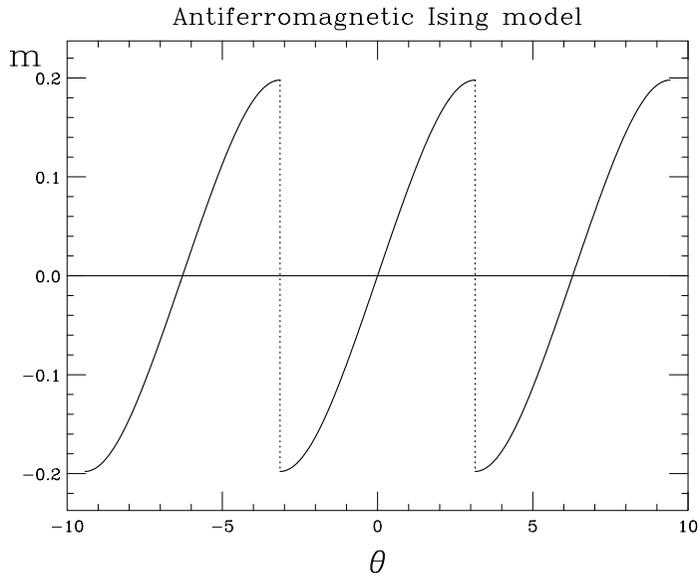


Fig. 2. Magnetization as a function of θ in the one-dimensional antiferromagnetic Ising model.

in the semi-classical approximation, as the solution of a given equation and the multiplicity of the solutions of this equation depends crucially on a certain inequality between quark masses. For realistic quark masses the solution would be unique, with periodicity 2π , and the vacuum energy density would be an analytic function of θ for every θ , including $\theta = \pi$.²¹⁾

There are however several possible explanations for the apparent contradiction between the chiral effective lagrangian results and ours, and we want just to enumerate some of them here. First the chiral effective lagrangian does not belong to the general class of models to which our results should apply since the quantized charge does not appear in it as an imaginary contribution to the euclidean action. Second the vacuum energy density obtained from the chiral effective lagrangian is the classical solution, i.e., it does not take into account quantum fluctuations which could change the vacuum structure; and third, higher order corrections to the chiral effective lagrangian could also change the vacuum energy density even at the classical level (see for instance Ref. 22)).

We want to stress also that the results reported in this article are complementary to the general analysis on spontaneous CP breaking developed by Creutz in Ref. 23). In fact our results would exclude some general ansatzes for the effective potential compatible with the symmetries considered by Creutz in Ref. 23) which drive to an order parameter analytical in θ .

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