QCD WITH A $\theta$-VACUUM TERM: A COMPLEX SYSTEM WITH A SIMPLE COMPLEX ACTION

V. AZCOITI* AND V. LALIENA
Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain
E-mail: azcoiti@azcoiti.unizar.es, laliena@posta.unizar.es

A. GALANTE
Dipartimento di Fisica dell’Università di L’Aquila, 67100 L’Aquila, Italy
E-mail: galante@lings.infn.it

We reanalyze in the first part of this paper the old question of P and CT realization in QCD. The second part is devoted to establish general results on the phase structure of this model in the presence of a $\theta$-vacuum term.

1 Introduction

Path integral formulation of Quantum Field Theories associates, in the more standard cases, a four-dimensional classical statistical mechanics system to a given quantum system. The euclidean partition function shows a well-defined Boltzmann weight, the correlation functions are the euclidean Green functions and the free energy density is equivalent to the vacuum energy density in the hamiltonian approach.

Even if the previous statement is true for almost all physically relevant systems, there are some notorious and important exceptions. The first relevant exception is lattice formulation of Quantum Chromodynamics at finite baryon density. Since the determinant of the Dirac operator at finite chemical potential is a complex number, the euclidean action of this model is complex. This is the most standard example of a complex system with a complex action. The meaning of "complex action" in this case is twofold: first, as previously discussed, the action is a complex number and second the complex part of the action involves fermionic degrees of freedom which are Grassmann variables.

It is well known that these two features have enormously delayed all attempts to analyze the behaviour of high density matter from first principles.

The second relevant exception to the equivalence between a quantum system and a classical statistical mechanics system is QCD with a topological term in the action. Due to the fact that the local density of topological charge

* TALK PRESENTED BY V. AZCOITI
picks-up a factor of $i$ under Wick rotation, the euclidean action of this model is also complex. This is an example of a complex system with a simple complex action. In fact even if the system is complex as opposite to simple, the complex part of the action is at least much simpler that the one which appears in QCD at finite baryon density since it involves only gauge degrees of freedom. It is therefore natural to think that if we have some hope to understand QCD at finite baryon density from first principles, we should be able to understand previously a simpler case of a complex system with a complex action: QCD with a topological term in the action. This was our last but not the least motivation to analyze this system.

This paper contains two differentiate parts. In the first one we will give a new look to the old Vafa-Witten theorem on the impossibility to break spontaneously parity and CT in vector-like theories as QCD and will show how an essential ingredient in the Vafa-Witten demonstration, the assumption that the free energy density exists in the presence of any external symmetry breaking field, requires the previous assumption that the symmetry is realized in the vacuum. In other words, the thesis of the theorem is in some sense assumed as an hypothesis.

The second part of the paper is devoted to the analysis of the phase structure of QCD with a $\theta$-vacuum term in the action. We will demonstrate a theorem which stays that if the $\theta$-vacuum term is relevant, either QCD has a phase transition at $\theta = \pi$ which breaks spontaneously parity or the free energy density has some non-analyticity at some $\theta < \pi$.

2 New look to the Vafa-Witten theorem.

Let us start this section by recalling the main ingredients and steps of Vafa-Witten theorem which stays that parity and CT cannot be spontaneously broken in vector-like parity conserving theories as QCD.

The theorem is based on the following two main points:

(i) The crucial observation that any arbitrary hermitian local order parameter $X$ for parity constructed from Bose fields have to be proportional to an odd power of the four indices antisymmetric tensor $\epsilon^{\mu\nu\rho\eta}$.

(ii) The assumption that the free energy density is well defined in the presence of a symmetry breaking source $\lambda X$.

The first of these two ingredients implies that any arbitrary order parameter $X$ should contain and odd number of time derivatives plus time components of the gauge field and should pick-up therefore a factor of $i$ under Wick rotation. This observation plus assumption (ii) makes the demonstration of the thesis actually very simple. In fact let $Z$ be the euclidean partition function
of QCD (or any parity conserving vector-like theory) in the presence of a local symmetry breaking source \( X \),

\[
Z = \int dA_\mu d\bar{\psi}d\psi \exp\left( -\int d^4x \left( \mathcal{L}(x) + i\lambda X(x) \right) \right)
\]  

(1)

where \( \mathcal{L}(x) \) is the standard QCD Lagrangian and \( X(x) \) is a real number since we have exhibited explicitly the factor of \( i \) which arises from Wick rotation. As can be seen in (1) the symmetry breaking term is a pure phase factor in the integrand of the partition function.

Since the determinant of the Dirac operator is positive definite in a vector-like theory as QCD, the presence of a pure phase factor in the integrand of the partition function can only decrease the value of \( Z \). Therefore the free energy density \( f(\lambda) \) defined as

\[
Z = e^{-V f(\lambda)}
\]

(2)

where \( V \) is the space-time volume, will increase with \( \lambda \). The vacuum energy density, which is given by the free energy density, will also increase with \( \lambda \) and therefore the symmetric vacuum will be stable under small perturbations.

Before going on in a deeper analysis let us say that it is actually surprising the fundamental role played in the mechanism previously discussed by the factor of \( i \) picked-up by the order parameter under Wick rotation. In fact the standard way to analyze spontaneous symmetry breaking is to add a symmetry breaking source to the symmetric action, compute the mean value of the order parameter, take the infinite volume limit and then the limit of vanishing symmetry breaking source. If at the end of this procedure we get a non-vanishing value for the order parameter the symmetry is spontaneously broken. But it is also well known that the symmetric action contains enough information on the realization of the symmetry in the vacuum. Indeed the analysis of the probability distribution function (p.d.f.) of the order parameter in the symmetric model has been extensively and successfully employed in the investigations on spontaneous symmetry breaking in spin systems like the Ising model, in spin-glass models in order to analyze the complicated structure of equilibrium states not connected by symmetry transformations, and more recently this formalism has also been extended to quantum systems with fermionic degrees of freedom.

But what is even more surprising is the contradictory result we obtain if we apply Vafa-Witten argumentation to the Ising model. The Ising model is not a quantum field theory but it verifies the main requirement in Vafa-Witten
theorem since the integration measure in this model is positive definite. If we add an imaginary external magnetic field to the hamiltonian of the Ising model and apply Vafa-Witten argumentation, we should conclude that the $Z_2$ symmetry of this model is not spontaneously broken. But this is obviously wrong since it is well known that in the low temperature phase the Ising model shows spontaneous magnetization. The solution to this paradox lies in the fact that the free energy density in the low temperature phase and for an imaginary magnetic field is not defined (it is singular on the imaginary axis of the complex magnetic field plane). The Lee-Yang zeroes of the partition function live on the imaginary axis and approach the origin with velocity $V$, the lattice volume, forbidding to get a well defined thermodynamical limit.

We will show in the following that this is not a pathology of the Ising model but a general feature of any model with a discrete $Z_2$ symmetry. In other words, we will show that to assume the euclidean free energy density $f(\lambda)$ is well defined in the presence of any external symmetry breaking source requires the previous assumption that the symmetry is realized in the vacuum.

To start the proof let us come back to equation (1) which defines the euclidean path-integral formula for the partition function. Using the p.d.f. of the order parameter $X$ we can write it as

$$Z(\lambda) = Z(0) \int d\tilde{X} P(\tilde{X}, V) e^{-i\lambda V \tilde{X}}$$

where $V$ in (3) is the space-time volume, $P(\tilde{X}, V)$ is the p.d.f. of $X$ at a given volume

$$P(\tilde{X}, V) = \frac{\int dA_\mu^a d\bar{\psi} d\psi e^{-\int d^4 x \mathcal{L}(x)} \delta \left( \tilde{X}(A_\mu^a) - \tilde{X} \right)}{\int dA_\mu^a d\bar{\psi} d\psi e^{-\int d^4 x \mathcal{L}(x)}}$$

and

$$\tilde{X}(A_\mu^a) = \frac{1}{V} \int d^4 x X(x)$$

Notice that, since the integration measure in (4) is positive or at least semi-positive definite, $P(\tilde{X}, V)$ is a true well normalized p.d.f.

Let us assume that parity is spontaneously broken. In the simplest case in which there is no an extra vacuum degeneracy due to spontaneous breakdown of some other symmetry, we will have two vacuum states as corresponds to a
discrete $Z_2$ symmetry. Since $X$ is an intensive operator, the p.d.f. of $X$ will be, in the thermodynamical limit, the sum of two $\delta$ distributions:

$$\lim_{V \to \infty} P(\tilde{X}, V) = \frac{1}{2}\delta(\tilde{X} - a) + \frac{1}{2}\delta(\tilde{X} + a) \quad (5)$$

At any finite volume, $P(\tilde{X}, V)$ will be some symmetric function ($P(\tilde{X}, V) = P(-\tilde{X}, V)$) developing a two peak structure at $\tilde{X} = \pm a$ and approaching (5) in the infinite volume limit.

Due to the symmetry of $P(\tilde{X}, V)$ we can write the partition function as

$$Z(\lambda) = 2Z(0)Re \int_0^\infty P(\tilde{X}, V)e^{-i\lambda V \tilde{X}} d\tilde{X} \quad (6)$$

and if we pick up a factor of $e^{-i\lambda Va}$

$$Z(\lambda) = 2Z(0)Re \left( e^{-i\lambda V a} \int_0^\infty P(\tilde{X}, V)e^{-i\lambda V (\tilde{X} - a)} d\tilde{X} \right) \quad (7)$$

which after simple algebra reads as follows:

$$\frac{Z(\lambda)}{2Z(0)} = \cos(\lambda Va) \int_0^\infty P(\tilde{X}, V) \cos(\lambda V (\tilde{X} - a)) d\tilde{X}$$

$$- \sin(\lambda Va) \int_0^\infty P(\tilde{X}, V) \sin(\lambda V (\tilde{X} - a)) d\tilde{X} \quad (8)$$

The relevant zeroes of the partition function in $\lambda$ can be obtained as the solutions of the following equation:

$$\cot(\lambda Va) = \frac{\int_0^\infty P(\tilde{X}, V) \sin(\lambda V (\tilde{X} - a)) d\tilde{X}}{\int_0^\infty P(\tilde{X}, V) \cos(\lambda V (\tilde{X} - a)) d\tilde{X}} \quad (9)$$

Let us assume for a while that the denominator in (9) is constant at large $V$. Since the absolute value of the numerator is bounded by 1, the partition function will have an infinite number of zeroes approaching the origin ($\lambda = 0$) with velocity $V$. In such a situation the free energy density does not converge in the infinite volume limit.

But this is essentially what happens in the actual case. In fact if we consider the integral in (9)
as a function of $\lambda V$ and $V$ it is easy to check that the derivative of $f(\lambda V, V)$ respect to $\lambda V$ vanishes in the large volume limit due to the fact that $P(\tilde{X}, V)$ develops a $\delta(\tilde{X} - a)$ in the infinite volume limit. At fixed large volumes $V$, $f(\lambda V, V)$ as function of $\lambda V$ is an almost constant non-vanishing function (it takes the value of $1/2$ at $\lambda V = 0$). The previous result on the zeroes of the partition function in $\lambda$ remains therefore unchanged; it generalizes the Lee-Yang theorem on the zeroes of the grand canonical partition function of the Ising model in the complex fugacity plane to any statistical model with a discrete $Z_2$ symmetry.

To illustrate this result with an example, let us take for $P(\tilde{X}, V)$ a double gaussian distribution

$$P(\tilde{X}, V) = \frac{1}{2} \left( \frac{V}{\pi} \right)^{1/2} \left( e^{-V(\tilde{X}-a)^2} + e^{-V(\tilde{X}+a)^2} \right)$$

which gives for the partition function

$$Z(\lambda) = Z(0) \cos(\lambda V a) e^{-\frac{2}{\lambda^2}V}$$

and for the mean value of the order parameter

$$<iX> = \frac{1}{2} \lambda + \tan(\lambda a V) a$$

The zeroes structure of the partition function is evident in (12) and consequently the mean value of the order parameter (13) is not defined in the thermodynamical limit. Notice also that if $a = 0$ (symmetric vacuum), the free energy density is well defined at any $\lambda$ and then Vafa-Witten’s argument applies.

2.1 Conclusions

We have shown in the previous section that an essential ingredient in the Vafa-Witten theorem on the impossibility to break spontaneously parity in a parity-conserving vector-like theory as QCD, the existence of the free energy density $f(\lambda)$ in the presence of any symmetry breaking external source $\lambda X$, does not work if the symmetry is spontaneously broken. The requirement that
the free energy density is well defined implies the previous assumption that
the symmetry is realized in the vacuum. This does not necessarily implies that
Vafa-Witten conjecture is wrong but at least a theorem on it is still lacking.

From a speculative point of view let us assume for a while that strong
interaction shows a weak spontaneous parity breaking. In such a case we would
expect a non-vanishing vacuum expectation value for the density of topological
charge at $\theta = 0$ and, as we have shown, the theory would be ill-defined at
$\theta \neq 0$. Actually this issue seems not very likely from a phenomenological point
of view, but this is not the only scenario in which the theory is ill-defined at
$\theta \neq 0$. In fact even if the symmetry is realized in the vacuum, the partition
function could have zeroes in $\theta$ approaching the $\theta = 0$ point with velocity
less than the space-time volume $V$ and also in this case the theory would be
ill-defined at $\theta \neq 0$.

A simple model which shows this feature is the lattice free-fermion theory,
the partition function of which shows zeroes on the imaginary axis of the
complex fermion-mass plane approaching the origin with velocity less than the lattice volume $V$. The chiral symmetry is realized in the free fermion
model and notwithstanding that, the zeroes structure of the partition function
forbids to define the theory at imaginary values of the fermion mass.

This speculative mechanism would provide us with a simple explanation
for the $\theta$-vacuum or strong CP problem: $\theta$ is zero because otherwise the
theory is ill-defined. As stated before this is a pure speculation at present but
we think it is worthwhile to investigate such an issue.

## 3 QCD at finite $\theta$. 

The partition function of QCD with a topological term in the action reads as
follows:

$$
Z = \int [dA^\mu_\nu] [d\psi] [d\bar{\psi}] \exp \left\{ - \int d^4x [\mathcal{L}(x) - \frac{i\theta}{16\pi^2} X(x)] \right\} 
$$

(14)

where $\mathcal{L}(x)$ is the standard QCD Lagrangian and

$$
X(x) = \epsilon_{\mu\nu\rho\sigma} \text{Tr} F^{\mu\nu} F^{\rho\sigma}
$$

(15)

is, up to a normalization constant, $1/16\pi^2$, the euclidean local density of
topological charge. The normalization constant has been chosen in such a
way that the topological charge

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$$\frac{1}{16\pi^2} \int d^4x X(x)$$

is an integer.

Assuming that the theory has a non-trivial $\theta$ dependence, we will show now the following theorem: "QCD with a topological term in the action, either breaks parity spontaneously at $\theta = \pi$, or has a phase transition at some critical $\theta_c$ less than $\pi$".

To start with the proof, let us write the partition function 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 by the proper topological phase:

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

(17)

where

$$g_V(n) = \int [dA_n^a] [d\psi] [d\bar{\psi}] \exp[-\int d^4x \mathcal{L}(x)]$$

(18)

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

$$p_V(n) = \frac{g_V(n)}{\sum_n g_V(n)}.$$ 

(19)

If we define the mean topological charge density

$$x_n = \frac{n}{V}$$

(20)

we can write the previous partition function as

$$Z_V(\theta) = \sum_{x_n} h_V(x_n) e^{i\theta V x_n},$$

(21)

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

Let the new $h_V(x)$ be a continuous interpolation of $h_V(x_n)$ and let us define a new function of $\theta$ in the following way:
\[ Z_{c,V}(\theta) = \int dx h_V(x) e^{i\theta V x}. \]  

(22) 

Summing up the "pseudo-partition" functions \( Z_{c,V}(\theta + 2\pi m) \) for all integers \( m \) we get

\[ \sum_m Z_{c,V}(\theta + 2\pi m) = \int dx h_V(x) e^{i\theta V x} \sum_m e^{i2\pi m V x}. \]  

(23) 

Using now the following representation of the periodic delta function:

\[ \sum_m e^{i2\pi m V x} = \frac{1}{V} \sum_m \delta(x - \frac{m}{V}), \]  

(24) 

we get the following identity:

\[ Z_V(\theta) = V \sum_m Z_{c,V}(\theta + 2\pi m), \]  

(25) 

which relates our QCD partition function \( Z_V(\theta) \) to the "pseudo-partition" functions \( Z_{c,V}(\theta + 2\pi m) \). The usefulness of this identity will become evident in a while. Before, let us come back to expression (21). Under a parity transformation, the density of topological charge, \( x_n \), changes sign, whereas \( h_V(x_n) \) is an even function of \( x_n \) since at \( \theta = 0 \) the QCD action is parity invariant. Taking also into account that the full topological charge \( Vx_n \) is an integer, we conclude that at \( \theta = \pi \) each term entering the sum of Eq. 21 is parity invariant. Therefore, at \( \theta = \pi \) the theory recovers the symmetry under parity transformations, and if the symmetry is also realized in the vacuum we must obtain a vanishing value for the expectation value of the topological charge density: \( \langle x \rangle = 0 \).

Using Eq. (22) we can write for the mean value of the density of topological charge:

\[ \langle x \rangle = \sum_m \langle x \rangle_{c,m} \left( \frac{Z_{c,V}(\theta + 2\pi m)}{\sum_n Z_{c,V}(\theta + 2\pi n)} \right), \]  

(26) 

with

\[ \langle x \rangle_{c,m} = \frac{\int dx x h_V(x) e^{i(\theta + 2\pi m) V x}}{\int dx h_V(x) e^{i(\theta + 2\pi m) V x}}, \]  

(27)
Since $x$ in (27) is a continuous variable (i.e. there is no symmetry forcing the numerator to be zero), we expect a non-vanishing value for $\langle x \rangle_{c,m}$ at $\theta = \pi$. However, it is simple to see that parity symmetry is realized at $\theta = \pi$ in a finite volume. In fact, the contribution of the $m = 0$ sector compensates the contribution of $m = -1$ in (24), the contributions $m = 1$ cancels that of $m = 2$, and so on. Therefore, at $\theta = \pi$ different sectors compensate to give $\langle x \rangle = 0$.

Equation (23) is valid for any value of $\theta$. At $\theta = 0$ it is simple to verify that in the infinite volume limit the sector $m = 0$ gives all the contribution to the partition function. This is a simple feature which follows from the fact that at $\theta = 0$ and in the infinite volume limit the exact solution for the free energy density is given by the saddle point solution, which is also the solution for the $m = 0$ sector. If this sector dominates for any value of $\theta$, we will get a first order phase transition at $\theta = \pi$, with a non-vanishing value of the topological charge density (remember the discussion following Eq. (27)), and the theory will undergo spontaneous parity breaking. Otherwise, there will be some critical value, $\theta_c$, at which other sectors start to give a contribution to the partition function, and in such a case we will get a phase transition at this $\theta_c$. On general grounds, we can say nothing about the number and order of phase transitions expected in this case.

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: the Ising model within an imaginary external magnetic field and a gaussian model.

### 3.1 The one-dimensional Ising model in an imaginary external magnetic field

In the previous demonstration we have not made use of any specific property of QCD, except the quantization of the topological charge. Therefore, the result applies to any model with a quantized topological charge which appears as an imaginary contribution to the euclidean action. A simple example of that is the one-dimensional Ising model in an imaginary external magnetic field. The hamiltonian of this model can be written as

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

(28)

where $J$ is the coupling constant between nearest neighbours, $k_B$ 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

\[ Z_N = \sum_{\{S\}} e^{F \sum_i S_i S_{i+1} + i\theta \sum_i S_i} \quad (29) \]

where \( F = J/k_BT \) and the sum is over all spin configurations.

For an even number of spins, the quantity \( \frac{1}{2} \sum_i S_i \) 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 "topological" charge. Furthermore, the theory has a \( Z_2 \) symmetry at \( \theta = 0 \) and \( \theta = \pi \) which, in the sense of this work, is the analogous of parity in QCD.

The transfer matrix technique allows to compute exactly the partition function defined in Eq. (29). The final result is

\[ Z_N = \lambda_+^N + \lambda_-^N, \quad (30) \]

where \( \lambda_\pm \) are the two eigenvalues of the transfer matrix, which are given by the following equation:

\[ \lambda_{\pm}(\theta) = e^F \cos \frac{\theta}{2} \pm \left( -e^{2F} \sin^2 \frac{\theta}{2} + e^{-2F} \right)^{1/2}. \quad (31) \]

We see that the external field \( \theta \) is an angle taking values between \(-\pi\) and \(\pi\), as expected.

Let us discuss first the simpler infinite temperature case. At \( T = \infty \), \( \lambda_- = 0 \) and \( \lambda_+ = 2\cos(\theta/2) \). The partition function has the simple form:

\[ Z_N = 2^N \cos^N(\theta/2), \quad (32) \]

from which it follows that the free energy density is

\[ f = \frac{1}{N} \log Z_N = \log 2 + \log \cos \frac{\theta}{2}. \quad (33) \]

For the mean magnetization we get

\[ \langle m \rangle = \left\langle \frac{1}{N} \sum_i S_i \right\rangle = i \tan \frac{\theta}{2}. \quad (34) \]
This last expression shows that a first order phase transition takes place at \( \theta = \pm \pi \), with divergent spontaneous magnetization. The origin of this phase transition is clarified by noticing that the sector \( m = 0 \) in Eqs. (25) and (26) dominates the thermodynamical limit for any \( \theta \).

The finite temperature case is somehow different. The eigenvalues of the transfer matrix, given by Eq. (31), are real and positive if

\[
\sin^2 \frac{\theta}{2} \leq e^{-4F}.
\]

(35)

In this case the free energy density has a well defined thermodynamical limit, and the mean magnetization is given by

\[
\langle m \rangle = i \frac{\sin(\theta/2)}{[e^{-4F} - \sin^2(\theta/2)]^{1/2}},
\]

(36)

which shows a first order phase transition with a divergent mean magnetization at

\[
\theta^\pm_c = \pm 2 \arcsin e^{-2F}.
\]

(37)

For \( \theta^+_c < \theta < \pi \) or \( -\pi < \theta < \theta^-_c \), the two eigenvalues of the transfer matrix are complex conjugate numbers. The partition function \( Z_N \) is real but not positive definite, and oscillates in sign with \( N \), making it impossible to define a thermodynamical limit. For instance, the mean magnetization does not converge as \( N \to \infty \). Thus, the theory is ill-defined in these intervals of \( \theta \). For \( \theta^-_c < \theta < \theta^+_c \), the sum in the right-hand side of Eqs. (25) and (26) is dominated by the term with \( m = 0 \), and the mean magnetization (36) is the analytic continuation of the saddle point solution obtained with real magnetic field.

3.2 Gaussian distribution.

The second illustrative example we want to discuss here are models 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. (21) has the form

\[
h_V(x_n) = e^{-V ax^2_n},
\]

(38)
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 behaviour far from the maximum can induce important changes in the $\theta$-dependence of the theory in the large $\theta$ regime (the previous example illustrates very well this point). 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 then

$$Z_V(\theta) = \sum_{x_n} e^{-Vax_n^2} e^{i\theta Vx_n}. \quad (39)$$

The pseudo-partition function $Z_{c,V}(\theta + 2\pi m)$ entering Eq. (25) can be analytically computed, and reads:

$$Z_{c,V}(\theta + 2\pi m) = \int dx e^{-Vax^2} e^{i(\theta+2\pi m)Vx} = \left(\frac{\pi}{aV}\right)^{1/2} e^{-\frac{1}{4\pi}(\theta+2\pi m)^2 V}. \quad (40)$$

Using Eq. (25) we can write

$$Z_V(\theta) = \left(\frac{\pi V}{a}\right)^{1/2} \sum_m e^{-\frac{1}{4\pi}(\theta+2\pi m)^2 V}, \quad (41)$$

and, if $|\theta| < \pi$, it is simple to verify that the free energy density $f(\theta)$ is given by

$$f(\theta) = \lim_{V \to \infty} \frac{1}{V} \log Z_V(\theta) = -\frac{1}{4a} \theta^2. \quad (42)$$

The $m = 0$ sector dominates for every $\theta$ between $-\pi$ and $\pi$. The vacuum expectation value of the density of topological charge, $\langle x \rangle$, is

$$\langle x \rangle = i\frac{\theta}{2a}, \quad (43)$$

and the model breaks spontaneously parity at $\theta = \pi$.
This simple model which, as we have seen, illustrates very well the theorem demonstrated in the first part of this section, has also further relevance. In fact, using a duality relation of gauge theories with a large number of colours and string theory on a certain space-time manifold, Witten has recently studied the dependence of pure gauge theories in four dimensions and has found Eqs. (42) and (43). Combining both results, we conclude that the probability distribution function of the topological charge density in pure SU($N$) gauge theory is gaussian in the large $N$ limit. It is interesting to note that also another analytically solvable model (although not physically relevant) has the same $\theta$ dependence: the quantum rotor in one dimension.

3.3 Conclusions.

We have demonstrated in the previous sections a theorem which states that if the $\theta$ dependence of QCD is non-trivial, either the theory has a first order phase transition at $\theta = \pi$ which breaks parity spontaneously, or the model shows a phase transition at some $\theta_c$ less than $\pi$. In the last case, we are not able to establish the order of the phase transition. Furthermore, the proof makes no use of any specific property of QCD, apart from the quantization of the topological charge. This implies that the result applies to any vector-like model with a quantized charge that appears as an imaginary contribution to the euclidean action.

To illustrate this result in practical cases and to get intuition on what we can expect in physical models, we have analyzed two simple examples: the one-dimensional Ising model in an imaginary external magnetic field, and a model in which the probability distribution function of the density of topological charge at $\theta = 0$ is assumed to be gaussian.

In the first case, we have found a first order phase transition with divergent spontaneous magnetization, at a critical imaginary magnetic field that depends on the temperature. At infinite temperature the transition is located at $\theta_c = \pi$ and the system breaks spontaneously its $Z_2$ symmetry at this $\theta$ value. At finite temperature the transition appears at $\theta_c < \pi$, and the theory is ill-defined for larger values of $\theta$ (modulo $2\pi$).

The model with gaussian distribution can be analyzed simply, and we have found a first order phase transition at $\theta_c = \pi$, which breaks spontaneously parity. The free energy density and the density of topological charge, which are quadratic and linear functions of $\theta$ respectively, agree exactly with the $\theta$-dependence of SU($N$) gauge theories in the large $N$ limit found recently by Witten. This implies that the topological charge density of this theory has a gaussian distribution at $\theta = 0$. 
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