Topology in the $SU(N_f)$ chiral symmetry restored phase of unquenched QCD and axion cosmology

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We investigate the topological properties of unquenched QCD on the basis of numerical results of simulations at fixed topological charge, recently reported by Borsanyi *et al.* We demonstrate that their results for the mean value of the chiral condensate at fixed topological charge are inconsistent with the analytical prediction of the large-volume expansion around the saddle point, and argue that the most plausible explanation for the failure of the saddle-point expansion is a vacuum energy density that is θ-independent at high temperatures, but surprisingly not too high ($T \sim 2T_c$), a result which would imply a vanishing topological susceptibility and the absence of all physical effects of the $U(1)$ axial anomaly at these temperatures. We also show that under a general assumption concerning the high-temperature phase of QCD, where the $SU(N_f)_A$ symmetry is restored, the analytical prediction for the chiral condensate at fixed topological charge is in very good agreement with the numerical results of Borsanyi *et al.*, all effects of the axial anomaly should disappear, the topological susceptibility and all the θ derivatives of the vacuum energy density vanish, and the theory becomes θ independent at any $T > T_c$ in the infinite-volume limit.

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I. INTRODUCTION

Understanding the role of the θ parameter in QCD and its connection with the strong-CP problem is one of the major challenges for high-energy theorists [1]. The aim of elucidating the existence of new low-mass, weakly interacting particles from a theoretical, phenomenological, and experimental point of view is intimately related to this issue. The light particle that has gathered the most attention has been the axion, predicted by Weinberg and Wilczek [2] and Wilczek [3] in the Peccei and Quinn mechanism [4] to explain the absence of parity and temporal-invariance violations induced by the QCD vacuum. The axion is one of the more interesting candidates to make up the dark matter of the Universe, and the axion potential, which determines the dynamics of the axion field, plays a fundamental role in this context. At high temperatures, the potential can be calculated in the dilute instanton gas model [5], but at medium and low temperatures interactions become nonperturbative, and a lattice QCD calculation is needed.

The calculation of the topological susceptibility in QCD is already a challenge, but calculating the complete potential requires a strategy to deal with the so-called sign problem, that is, the presence of a highly oscillating term in the path integral. Indeed, Euclidean lattice gauge theory, our main nonperturbative tool for QCD studies from first principles, has not been able to help us much because of the imaginary contribution to the action coming from the θ term, which prevents the applicability of the importance sampling method [6]. This is the main reason why the only progress in the analysis of the θ dependence of the vacuum energy density in pure gauge QCD, from first principles, reduces to the computation of the first few coefficients (up to order θ^6) in the expansion of the free-energy density in powers of θ [7–9], and the maximum temperature at which quenched simulations seem to give reliable results for the topological susceptibility is of the order of $1.5T_c$ [10–12], with T_c the critical temperature for the chiral symmetry restoration phase transition. The situation in full QCD with dynamical fermions is, on the other hand, even worse [13–15].

The QCD axion model relates the topological susceptibility χ_T at $\theta = 0$ with the axion mass m_a and decay constant f_a through the relation $\chi_T = m_a^2 f_a^2$. The axion mass is, on the other hand, an essential ingredient in the calculation of the axion abundance in the Universe. Therefore, a precise computation of the temperature dependence of the topological susceptibility in QCD becomes of primordial interest in this context. This is the reason why several calculations of the topological susceptibility in unquenched QCD have been published recently [13–15].

The authors of Ref. [13] explore $N_f = 2 + 1$ QCD in a range of temperatures, from T_c to around $4T_c$, and their results for the topological susceptibility differ strongly, both in the size and in the temperature dependence, from the dilute instanton gas prediction, giving rise to a shift of the axion dark-matter window of almost 1 order of magnitude with respect to the instanton computation. The authors of Ref. [14], however, observe in the same model very distinct temperature dependences of the topological susceptibility in the ranges above and below

250 MeV; though for temperatures above 250 MeV, the dependence is found to be consistent with the dilute instanton gas approximation, at lower temperatures the falloff of topological susceptibility is milder. On the other hand, a novel approach is proposed in Ref. [15], i.e., the fixed Q integration, based on the computation of the mean value of the gauge action and chiral condensate at fixed topological charge Q; they find a topological susceptibility many orders of magnitude smaller than that of Ref. [13] in the cosmologically relevant temperature region.

We want to show in this paper that an analysis of some of the numerical results reported in Ref. [15] concerning the mean value of the chiral condensate at fixed topological charge suggest that the vacuum energy density is θ independent at high temperatures, but surprisingly not too high ($T \sim 2T_c$); this is a result which would imply a vanishing topological susceptibility and the absence of all physical effects of the $U(1)$ axial anomaly at these temperatures. Since our analysis is based on the computation of physical quantities at fixed topological charge, we summarize some peculiar features of such a computation and derive an expression for the ratio of partition functions in different topological sectors in Sec. II. In Sec. III we show, provided that the vacuum energy density has a nontrivial θ dependence, that the difference of gauge actions and of chiral condensates between the Q and vanishing topological sectors are in both cases of the order of the inverse lattice volume $\frac{1}{V_x L_t}$ and proportional to the square of the topological charge Q. In this section we also compare our analytical results with the numerical results reported in Ref. [15]. The absence of the typical effects of the $U(1)_A$ anomaly in the chiral symmetry restored phase of QCD at high temperatures was suggested years ago [16,17], and investigated later on in [18–27]. In Sec. IV we show, under very general assumptions, that all effects of the axial anomaly should disappear in the high-temperature phase of QCD, where the $SU(N_f)_A$ symmetry is restored. The topological susceptibility and all the θ derivatives of the vacuum energy density should vanish and the theory should become θ independent. Our conclusions are reported in Sec. V.

II. QCD WITH A θ TERM

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. In particle physics, these models describe particle interactions with a CP-violating term. The inclusion of this term in the QCD Lagrangian was the result of the discovery of the $U(1)$ axial anomaly, which solved the $U(1)_A$ problem but generated a new problem, that of strong CP.

The Euclidean continuum Lagrangian of N_f flavors QCD with a θ term is

$$L = \sum_f L_F^f + \frac{1}{4} F_{\mu\nu}^a(x) F_{\mu\nu}^a(x) + i\theta \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x), \tag{1}$$

with L_F^f the fermion Lagrangian for the f flavor, and

$$Q = \frac{g^2}{64\pi^2} \int d^4x \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x) \tag{2}$$

is the topological charge of the gauge configuration, which takes integer values.

In this section we summarize a few interesting features, some of them well known, of QCD with a topological term in the action. One of these features concerns the fact that the mean value of any intensive operator in QCD at $\theta = 0$ can be computed in any fixed topological sector [28,29], in particular in the $Q = 0$ topological sector. Even if this result seems a paradox, because the zero charge topological sector is free from the $U(1)_A$ anomaly and breaks spontaneously chiral symmetry, we will show how one can reconciliate the absence of the $U(1)_A$ anomaly with a finite nonvanishing mass for the η meson. We will discuss separately the one-flavor model and the case of several flavors, and will derive a expression for the ratio of partition functions in different topological sectors, which will be useful in the next section.

A. The one-flavor model

Concerning the one-flavor model, where the only axial symmetry is an anomalous $U(1)$ symmetry, the standard wisdom on the vacuum structure of this model in the chiral limit is that it is unique at each given value of θ, the θ vacuum. Indeed, the only plausible reason to have a degenerate vacuum in the chiral limit would be the spontaneous breakdown of chiral symmetry, but because it is anomalous, there is no symmetry. Furthermore, in contrast to what happens when chiral symmetry is spontaneously broken, the infinite volume limit and the chiral limit commute. In fact, due to the chiral anomaly, the model shows a mass gap in the chiral limit and, therefore, all correlation lengths are finite in physical units.

An elegant realization of all these ideas is the Leutwyler and Smigla (L-S) approach [30]. This approach is based, for the one-flavor model, on the assumption that the vacuum energy or free-energy density can be expanded in powers of the fermion mass m, treating the quark mass term as a perturbation. Indeed, as previously stated, the spectrum of the one-flavor model, due to the chiral anomaly, does not contain massless particles and, therefore, the perturbation series in powers of the fermion mass m should not give rise to infrared divergences. This expansion will be then an ordinary Taylor series

$$-E(m,\theta) = -E_0 + \Sigma m cos\theta + O(m^2), \tag{3}$$

giving rise to the following expansions for the scalar and pseudoscalar condensates:

$$\langle \bar{u}u \rangle = \Sigma cos\theta + O(m), \tag{4}$$

$$\langle i\bar{u}\gamma_5 u \rangle = \Sigma sin\theta + O(m). \tag{5}$$

The resolution of the $U(1)$ axial problem is obvious in this approach. Indeed, the expression for the free-energy density (3) tell us that the topological susceptibility χ_T has the following expansion:

$$\chi_T = \Sigma m cos\theta + O(m^2), \tag{6}$$

and then the divergence in the chiral limit of the first term in the right-hand side of the equation relating the pseudoscalar susceptibility

$$\chi_p = \int \langle i\bar{u}(x)\gamma_5 u(x) i\bar{u}(0)\gamma_5 u(0)\rangle d^4x$$

with the chiral condensate and χ_T

$$\chi_p = \frac{\langle \bar{u}u \rangle}{m} - \frac{\chi_T}{m^2} \tag{7}$$

is compensated with the divergence of second term in this equation, giving rise to a finite pseudoscalar susceptibility or, equivalently, a finite mass for the $\bar{u}\gamma_5 u$ meson.

All these features can be understood in simple words. Because of the chiral anomaly, a nonvanishing value of the chiral condensate does not break any symmetry. The Goldstone theorem is not fulfilled because there is no spontaneous symmetry breaking.

The L-S formalism was developed in the continuum. However, there is a lattice regularization, the Ginsparg-Wilson (G-W) fermions [31] from which the overlap fermions [32] are an explicit realization, which shares with the continuum all essential ingredients and gives at the same time mathematical rigor to all developments. Indeed G-W fermions have a $U(1)$ anomalous symmetry [33], good chiral properties, a quantized topological charge, and allow us to establish and exact index theorem on the lattice [34]. Furthermore G-W fermions, in contrast to Wilson fermions, are free from phases where parity and flavor symmetries are spontaneously broken [35]. We will use this lattice regularization in what follows.

With this in mind we can write for the free-energy density E, scalar S and pseudoscalar P condensates, pseudoscalar susceptibility χ_p, and topological susceptibility χ_T the same expressions as in the L-S approach,

$$-E(\beta, m, \theta) = -E_0(\beta) + \Sigma m cos\theta + O(m^2), \tag{8}$$

$$\langle S \rangle = \Sigma cos\theta + O(m), \tag{9}$$

$$\langle P \rangle = \Sigma sin\theta + O(m), \tag{10}$$

$$\chi_T = \Sigma m cos\theta + O(m^2), \tag{11}$$

$$\chi_p = \frac{\langle S \rangle}{m} - \frac{\chi_T}{m^2}, \tag{12}$$

where these expressions are now valid at finite lattice spacing a and finite lattice volume V, and Σ depends on both parameters with a finite nonvanishing value in the infinite volume limit. β is the inverse gauge coupling and we omit the β dependence of Σ for simplicity.

The partition function of the model can be written as a sum over all topological sectors Q of the partition function in each topological sector times a θ-phase factor as follows:

$$Z(\theta) = \sum_Q Z_Q e^{i\theta Q}, \tag{13}$$

where Q takes all integer values, and it is bounded at finite volume by the number of degrees of freedom.

At large lattice volume V the partition function should behave as

$$Z(\theta) = e^{-VE(\beta,m,\theta)} \tag{14}$$

with $E(\beta, m, \theta)$ given by (8). On the other hand, the mean value of any intensive operator O, as for instance the scalar and pseudoscalar condensates or any correlation function, in a given topological sector Q, can be computed as follows:

$$\langle O \rangle_Q = \frac{\int d\theta \langle O \rangle_\theta Z(\theta, m) e^{-i\theta Q}}{\int d\theta Z(\theta, m) e^{-i\theta Q}}. \tag{15}$$

Because the vacuum energy density, as a function of θ, has its absolute minimum at $\theta = 0$, Eqs. (8) and (15) tell us that the mean value of any intensive operator at $\theta = 0$ and nonvanishing fermion mass can be computed in any fixed topological sector. Indeed, Eq. (15) gives in the infinite lattice volume limit the following relation:

$$\langle O \rangle_Q = \langle O \rangle_{\theta=0}. \tag{16}$$

We can apply Eq. (16) to the computation of the pseudoscalar correlation function $\langle P(x)P(0)\rangle_{\theta=0}$ by computing it in the vanishing charge topological sector. However, this sector is anomaly free, and breaks spontaneously chiral symmetry in order to give a nonvanishing value Σ for the chiral condensate in the chiral limit. The pseudoscalar meson susceptibility diverges and the Goldstone theorem should tell us that the pseudoscalar meson is massless in the chiral limit. The loophole in this argument is that in systems with a global constraint, the divergence of the susceptibility does not necessarily imply a divergent correlation length. Indeed, the susceptibility must be computed by integrating out the correlation function over all distances, and then taking the infinite-volume limit, in this order. In systems with a global constraint, the infinite-volume limit and the space integral of the correlation function do not necessarily commute. A very simple example of that is the Ising model at infinite temperature with an even number of spins and with vanishing full magnetization as a global constraint. In such a case, one has for the spin-spin correlation function

$$\langle s_i^2 \rangle = 1$$
$$\langle s_i s_j \rangle = -\frac{1}{(V-1)}.$$

The integral of the infinite-volume limit of the correlation function is equal to 1, whereas the infinite volume limit of the integrated correlation function vanishes. The correlation function has a contribution of order $1/V$ that violates cluster at finite volume and vanishes in the infinite-volume limit, but that gives a finite contribution to the integrated correlation function. This example, even if very simple, is illustrative because this is in fact what happens for the pseudoscalar correlation function.

Coming back to QCD with a θ term, the standard wisdom on this model is that it has no phase transition at $\theta = 0$. Then we can expand the pseudoscalar correlation function in powers of the θ angle as follows:

$$\langle P(x)P(0)\rangle_\theta = \langle P(x)P(0)\rangle_{\theta=0} + h(x, m_u)\theta^2 + O(\theta^4), \tag{17}$$

where

$$h(x, m_u) = \langle S(x)S(0)\rangle_{\theta=0} - \langle P(x)P(0)\rangle_{\theta=0} + O(m_u). \tag{18}$$

The vacuum energy density (8) can also be expanded in powers of θ as

$$-E(\beta, m_u, \theta) = -E_0(\beta, m_u) - \frac{1}{2}\chi_T(\beta, m_u)\theta^2 + O(\theta^4) \tag{19}$$

with

$$\chi_T(\beta, m_u) = m_u \Sigma + O(m_u^2). \tag{20}$$

Taking into account Eqs. (16) and Eqs. (17)–(19) and making an expansion around the saddle-point solution, we can write the following equation for the pseudoscalar correlation function in the zero-charge topological sector:

$$\langle P(x)P(0)\rangle_{Q=0} = \langle P(x)P(0)\rangle_{\theta=0} + \frac{1}{V}\frac{\langle S(x)S(0)\rangle_{\theta=0} - \langle P(x)P(0)\rangle_{\theta=0} + O(m_u)}{\chi_T} + O\left(\frac{1}{V^2}\right). \tag{21}$$

Equation (21) shows, as in the simple Ising model case, a violation of cluster at finite volume for the pseudoscalar correlation function in the zero-charge topological sector. In the infinite-volume limit, the pseudoscalar correlation function in the zero-charge topological sector and in QCD at $\theta = 0$ agree, as expected. Concerning susceptibilities we can write, by integrating out Eq. (21) and taking the infinite volume limit, the following relation:

$$\chi_{p,Q=0} = \chi_p + \frac{\Sigma^2 + O(m_u)}{\chi_T} \tag{22}$$

where we have made use of the fact that in the infinite-volume limit intensive operators do not fluctuate,

$$\left\langle \left(\frac{1}{V}\sum_x S(x)\right)^2 \right\rangle = \left\langle \frac{1}{V}\sum_x S(x) \right\rangle^2$$
$$\left\langle \left(\frac{1}{V}\sum_x P(x)\right)^2 \right\rangle = \left\langle \frac{1}{V}\sum_x P(x) \right\rangle^2.$$

The dominant contribution of the second term in Eq. (22) in the chiral limit diverges with the quark mass as Σ/m_u, whereas

$$\chi_{p,Q=0} = \frac{\langle S(x)\rangle}{m_u}.$$

Combining these results we get, notwithstanding the pseudoscalar susceptibility diverges in the zero-charge sector in the chiral limit, that the pseudoscalar susceptibility in one-flavor QCD is finite and the pseudoscalar meson is massive. The pseudoscalar susceptibility in the $Q = 0$ sector diverges in the chiral limit not because of a divergent correlation length but as a consequence of the cluster-violating contributions to the pseudoscalar correlation function (21), which are singular at $m = 0$ and of order $\frac{1}{V}$, and which give a finite singular contribution to $\chi_{p,Q=0}$.

To conclude the discussion on the one-flavor model, we want to remark that the validity of the commutation of the infinite-volume limit and the chiral limit in this model does not apply to the zero-charge topological sector. Indeed, as previously stated, the zero-charge topological sector breaks spontaneously chiral symmetry, and even if all correlation lengths are finite in this sector, there are divergent susceptibilities in the chiral limit. We have seen that the pseudoscalar susceptibility diverges in this sector, but also the scalar susceptibility χ_s at vanishing quark mass can be computed as

$$\chi_{s,Q=0,m_u=0} = \frac{1}{2}(\chi_{s,m_u=0} + \chi_{p,m_u=0}) + \frac{V}{2}\Sigma^2, \qquad (23)$$

which shows explicitly the divergence with the lattice volume V, and makes the perturbative expansion of the chiral condensate in powers of m_u ill defined in the infinite-volume limit.

B. Several flavors

QCD with several flavors shows some important differences with respect to the one-flavor case. The model also suffers from the chiral anomaly but has a spontaneously broken $SU(N_f)$ chiral symmetry in the chiral limit at any temperature below the critical temperature of the chiral transition T_c. There are divergent correlation lengths for $T < T_c$ in this limit and, in contrast to the one-flavor case, the infinite-volume limit and the chiral limit do not commute if $T < T_c$. However, the essential features previously described for the one-flavor model still work in the several-flavors case. Equation (12) reads now

$$\chi_p = \frac{\langle S \rangle}{m} - N_f^2 \frac{\chi_T}{m^2}, \qquad (24)$$

where χ_p stands now for the flavor singlet pseudoscalar susceptibility and S is the flavor singlet scalar condensate. The vacuum energy density can also be expanded in this case in powers of the θ angle as

$$E(\beta, m_f, \theta) = E_0 - \frac{1}{2}\chi_T(\beta, m_f)\theta^2 + O(\theta^4), \qquad (25)$$

and Eqs. (13)–(16) also work for several flavors.

Let us write the expression, which we will use in the following, for the ratio of the partition functions in the Q topological sector Z_Q and in the vanishing topological sector Z_0

$$\frac{Z_Q}{Z_0} = \frac{\int d\theta e^{-iQ\theta} Z(\theta, m)}{\int d\theta Z(\theta, m)}, \qquad (26)$$

and its expansion around the saddle-point solution

$$\frac{Z_Q}{Z_0} = 1 - \frac{1}{V_x L_t}\frac{Q^2}{2\chi_T} + O\left(\frac{1}{V^2}\right), \qquad (27)$$

where V_x is the spatial lattice volume and L_t the number of lattice points in time direction. Equation (27) implies that all topological sectors have the same probability in the infinite spatial volume limit at any temperature $T = 1/L_t$. Otherwise, the saddle-point expansion breaks down, the most plausible reason for which being that the vacuum energy density (25) is θ independent.

III. THE FINITE-TEMPERATURE CHIRAL TRANSITION

We want to explore in this section the physical consequences of Eq. (27) on the temperature dependence of the topological susceptibility.

Taking the logarithm in (27) we get

$$\log \frac{Z_Q}{Z_0} = -\frac{1}{V_x L_t}\frac{Q^2}{2\chi_T} + O\left(\frac{1}{V^2}\right) \qquad (28)$$

and the following expressions for the logarithmic derivatives with respect to the inverse-square gauge coupling β and fermion masses m_f:

$$\langle S_g \rangle_Q - \langle S_g \rangle_{Q=0} = \frac{Q^2}{V_x L_t}\frac{1}{2\chi_T^2}\frac{\partial \chi_T}{\partial \beta} + O\left(\frac{1}{V^2}\right) \qquad (29)$$

$$\left\langle \sum_x S_f(x) \right\rangle_Q - \left\langle \sum_x S_f(x) \right\rangle_{Q=0} = \frac{Q^2}{V_x L_t}\frac{1}{2\chi_T^2}\frac{\partial \chi_T}{\partial m_f} + O\left(\frac{1}{V^2}\right), \qquad (30)$$

where S_g and $S_f(x)$ in (29) are the lattice pure gauge action and the scalar chiral condensate, respectively.

There are two remarkable properties of the difference of gauge actions and of chiral condensates between the Q and vanishing topological sectors in Eqs. (29) and (30): they are of the order of the inverse lattice volume $\frac{1}{V_x L_t}$ and proportional to the square of the topological charge Q in both cases.

The numerical results for $\langle S_g \rangle_Q - \langle S_g \rangle_{Q=0}$ and $\langle \sum_x S_f(x) \rangle_Q - \langle \sum_x S_f(x) \rangle_{Q=0}$ reported in Ref. [15] show a finite nonvanishing contribution in the infinite volume limit, linear in $|Q|$ for both quantities. These results have been obtained from numerical simulations of lattice QCD with $N_f = 3 + 1$ staggered dynamical quarks at $T \sim 5T_c$ and $N_f = 2 + 1$ overlap fermions, the last in a range of temperatures running from $2T_c$ to $4T_c$ [15], and also in the quenched model [36]. Furthermore, the numerical results of Ref. [15] show a value of $\langle \sum_x S_f(x) \rangle_{Q=1} - \langle \sum_x S_f(x) \rangle_{Q=0}$,

$$\left\langle \sum_x S_f(x) \right\rangle_{Q=1} - \left\langle \sum_x S_f(x) \right\rangle_{Q=0} \approx \frac{1}{m_f}, \qquad (31)$$

independent of the temperature, in the range of temperatures reported (300–650 MeV).

Summarizing, the results reported in [15] for the difference of the gauge action and of the chiral condensate between the Q and vanishing topological sectors, obtained from numerical simulations of QCD at $T > T_c$, are in contradiction with the corresponding results obtained from the expansion around the saddle point [(29) and (30)], which should hold in the large-volume limit.

There are only two plausible explanations for such a contradiction:

(i) The results of Ref. [15] are afflicted from strong volume corrections.

(ii) The saddle-point expansion fails to reproduce the correct behavior of physical quantities in the large-volume limit.

Because the authors of Ref. [15] exclude large finite-size corrections from their numerical analysis of the difference of the gauge action and of the chiral condensate between the Q and vanishing topological sectors (see Figs. S19 and S22 of [15]), the only plausible explanation is the failure of the expansion around the saddle point. However, the only reason for the failure of the saddle-point expansion is that the main ingredient of this expansion, the fact that $Z(\theta)$ defines in (26) an integration measure extremely sharp around $\theta = 0$, does not work. Because $Z(\theta) = e^{-V_x L_t E(\beta, m_f, \theta)}$ and $E(\beta, m_f, \theta)$ has its absolute maximum at $\theta = 0$ for any nonvanishing value of the fermion mass m_f and gauge coupling β, we should conclude, as previously stated, that the vacuum energy density is θ independent at high temperatures, but surprisingly not too high ($T \sim 2T_c$). A θ-independent vacuum energy density for physical temperatures above a given temperature T_{ch} would imply a vanishing topological susceptibility and the absence of all physical effects of the $U(1)$ axial anomaly at these temperatures.

Years ago Cohen [16,17] showed, assuming the absence of the zero mode's contribution, that all the disconnected contributions to the two-point correlation functions in the $SU(2)_A$ chiral symmetry restored phase at high temperatures vanish in the chiral limit. The main conclusion of this work was that the eight scalar and pseudoscalar mesons $\sigma, \bar{\pi}, \eta, \bar{\rho}$, should have the same mass in the chiral limit, the typical effects of the $U(1)_A$ anomaly being absent in this phase. This issue has been investigated both analytically and with numerical simulations in [18–27]. In particular, Aoki and collaborators have reported numerical results from simulations of QCD with overlap fermions [23,25] which show a degeneracy of the $\bar{\pi}$ and η correlators. In addition, they have also shown in [24], by studying multipoint correlation functions in various channels, that the $U(1)_A$ anomaly becomes invisible in susceptibilities of scalar and pseudoscalar mesons in the $SU(2)_A$ chiral symmetric phase of QCD with two overlap quarks.

In the next section we will argue that the effects of the chiral anomaly on the meson spectrum, and in any physical observable, should disappear in the high-temperature $SU(N_f)_A$ chiral symmetric phase of QCD.

IV. THE RESTORATION OF THE $U(1)_A$ SYMMETRY AT ANY $T > T_c$

In this section we want to show, on very general grounds, how all effects of the axial anomaly should disappear in the high-temperature phase of QCD, where the $SU(N_f)_A$ symmetry is restored. The topological susceptibility and all the θ derivatives of the vacuum energy density should vanish and the theory should become θ independent.

The only general assumption of this section is that in the high-temperature phase of QCD, where the $SU(N_f)_A$ symmetry is restored, the spectrum shows a mass gap even in the chiral limit. All correlation lengths are finite in physical units, no symmetry is spontaneously broken, the model is free from infrared divergences, and the perturbative expansion of the vacuum energy density and of the chiral condensate in powers of the quark mass converges for every θ (phase transitions in θ are not expected at $T > T_c$ [9,37]). A finite spatial lattice volume of linear size much larger than the inverse mass gap should be enough to reproduce the correct physical results, and in contrast to what happens in the low-temperature broken phase, the infinite-volume limit and the chiral limit should commute. The situation is similar to that of the one-flavor model previously discussed, where the chiral anomaly and, therefore, the absence of spontaneous chiral symmetry breaking was responsible for the mass gap in the spectrum of this model. However, in contrast to the one-flavor case, the zero-charge topological sector does not show spontaneous symmetry breaking, and all susceptibilities are finite in the chiral limit in this sector. This suggests that the validity of the perturbative expansion in powers of the quark mass m, and of the commutation of the infinite volume limit and the chiral limit, applies also to this sector; we will make use of this in what follows.

We will first discuss the two-flavor case and will comment on the extension of the results to $N_f \geq 3$. We will also show that Eq. (31) holds in the chiral symmetry restored phase, up to order-m_f corrections, a result which, as previously stated, has been observed in the numerical simulations reported in [15] at $T = 2T_c$. We work, as throughout this paper, in a lattice with a fermion regularization that, as the overlap fermions, obey the Ginsparg-Wilson relation.

A. The two-flavor model

To fix the notation let $S(x) = S_u(x) + S_d(x)$ and $P(x) = P_u(x) + P_d(x)$ be the sum of the up and down scalar and pseudoscalar condensates, respectively, let $\chi_{s,m=0,V}$ and $\chi_{p,m=0,V}$ be the flavor singlet scalar and pseudoscalar susceptibilities at $m = m_u = m_d = 0$, and let finite lattice volume $V = L_s^3 L_t$. Taking into account that $S(x)$ and $P(x)$ transform like a vector under $U_A(1)$ chiral anomalous rotations, we can write for the expansion of the mean value of the chiral condensate in powers of m

$$\langle S(x)\rangle_\theta = \chi_{s,m=0,V} m - \sin^2\frac{\theta}{2}(\chi_{s,m=0,V} - \chi_{p,m=0,V})m + O(m^3), \tag{32}$$

which gives the following expression for the vacuum energy density:

$$-E_V(\beta,m,\theta) = -E_{0,V}(\beta) + \frac{1}{2}\chi_{s,m=0,V}m^2 - \frac{1}{2}\sin^2\frac{\theta}{2}(\chi_{s,m=0,V} - \chi_{p,m=0,V})m^2 + O(m^4), \tag{33}$$

where $E_{0,V}(\beta)$ is the vacuum energy density at $m = 0$, which depends only on the inverse gauge coupling β.

Equation (33) gives for the topological susceptibility at $\theta = 0$ the following relation with the scalar and pseudoscalar flavor-singlet susceptibilities:

$$\chi_{T,V} = \frac{m^2}{4}(\chi_{s,m=0,V} - \chi_{p,m=0,V}) + O(m^4), \tag{34}$$

which is of the order of m^2, as expected.

Equations (32) and (33) allow us to write the following expansion in powers of m for the mean value of the chiral condensate in the $Q = 0$ topological sector:

$$\langle S(x)\rangle_{Q=0} = \chi_{s,m=0,V}m - \frac{1}{2}(\chi_{s,m=0,V} - \chi_{p,m=0,V})m + O(m^3). \tag{35}$$

As previously discussed, the large lattice volume expansion around the saddle point predicts, provided that the vacuum energy density shows a nontrivial θ dependence, that the chiral condensate in any fixed topological sector equals the chiral condensate in the full theory at $\theta = 0$, in the large-volume limit, up to corrections of the order of $\frac{1}{V}$. Then the only way to keep the validity of the expansion of the chiral condensate and the vacuum energy density in powers of the quark mass m is that $\chi_{s,m=0,V} - \chi_{p,m=0,V}$ is $O(\frac{1}{V})$,

$$\chi_{s,m=0,V} - \chi_{p,m=0,V} \sim O\left(\frac{1}{V}\right). \tag{36}$$

Equation (36) implies that the topological susceptibility (34) vanishes, the scalar and pseudoscalar susceptibilities are equal in the chiral limit, and, therefore, the eight scalar and pseudoscalar mesons $\sigma, \bar{\pi}, \eta, \bar{\rho}$ should have the same mass in this limit.

The analysis here performed can be extended to higher orders in the expansions (32)–(35), obtaining as a result new conditions, analogous to (36), that show that the theory should be θ independent in the infinite-volume limit and that all the effects of the chiral anomaly are missed.

There is a simpler way to understand all these features. The vacuum energy density can be parameterized as follows:

$$E_V(\beta,m,\theta) - E_V(\beta,m,0) = m^2\theta^2 f(\beta,m,\theta^2), \tag{37}$$

with $f(\beta,m,\theta^2) > 0$ for every $\theta \in (-\pi,\pi]$, since $\theta = 0$ is assumed to be the only absolute minimum of the vacuum energy density. It is an even function of θ ($f(\beta,m,\theta^2)$ is also an even function of m in the two-flavor model) that vanishes at $m = 0$. The subtracted full chiral condensate $\langle\sum_x S(x)\rangle_{\theta=0} - \langle\sum_x S(x)\rangle_{Q=0}$ is, on the other hand, finite in the infinite-volume limit, and can be computed as follows:

$$\left\langle\sum_x S(x)\right\rangle_{\theta=0} - \left\langle\sum_x S(x)\right\rangle_{Q=0} = V_x L_t \frac{\int d\theta(2mf(\beta,m,\theta^2) + m^2\partial_m f(\beta,m,\theta^2))\theta^2 e^{-V_x L_t m^2\theta^2 f(\beta,m,\theta^2)}}{\int d\theta e^{-V_x L_t m^2\theta^2 f(\beta,m,\theta^2)}}, \tag{38}$$

which obviously vanishes at $m = 0$.

We can compute the subtracted full chiral condensate at any nonvanishing quark mass m by doing the saddle-point expansion of (38) and the final result for the dominant contribution in the $m \to 0$ limit is

$$\left\langle\sum_x S(x)\right\rangle_{\theta=0} - \left\langle\sum_x S(x)\right\rangle_{Q=0} = \frac{1}{m}. \tag{39}$$

Then, if we want to keep the validity of the expansion of the vacuum energy density in powers of the quark mass m, and of the commutation of the infinite-volume limit and the chiral limit, we need to invalidate the saddle-point expansion; this requires that the θ-dependent part of the vacuum energy density (37) be at least of the order of $\frac{1}{V}$.

We can also compute the mean value of the chiral condensate in the $Q = 1$ topological sector under this condition [or condition (36)]. The final result is

$$m\langle S(x)\rangle_{Q=1} = \chi_{s,m=0,V}m^2 + \frac{1}{V}(2 + O(m^2)), \tag{40}$$

which gives for the difference between the full condensates in the $Q = 1$ and $Q = 0$ topological sectors the following expression:

$$m\left(\left\langle\sum_x(S_u(x)+S_d(x))\right\rangle_{Q=1} - \left\langle\sum_x(S_u(x)+S_d(x))\right\rangle_{Q=0}\right) = 2 + O(m^2). \tag{41}$$

B. Three or more flavors

The generalization of the results of the previous subsection to $N_f \geq 3$ is straightforward but has some peculiar features which we want to remark.

In the two-flavor model the scalar $\chi_{s,m=0,V}$ and pseudoscalar $\chi_{p,m=0,V}$ susceptibilities in the chiral limit get contributions from the $Q = 0$ and $Q = 1$ topological sectors. The $Q = 0$ sector is free from the anomaly, and then gives the same contribution to both susceptibilities, but the $Q = 1$ sector contributions to $\chi_{s,m=0,V}$ and $\chi_{p,m=0,V}$ are opposite. For $N_f \geq 3$, however, only the $Q = 0$ sector gives a contribution to the scalar $\chi_{s,m=0,V}$ and pseudoscalar $\chi_{p,m=0,V}$ susceptibilities in the chiral limit and, therefore, we get

$$\chi_{s,m=0,V} = \chi_{p,m=0,V}, \quad \text{if } N_f \geq 3. \tag{42}$$

The expansion of the mean value of the chiral condensate in powers of m for $N_f = 3$,

$$\langle S(x)\rangle_\theta = \chi_{s,m=0,V}m - \sin^2\frac{\theta}{3}(\chi_{s,m=0,V} - \chi_{p,m=0,V})m + O(m^2), \tag{43}$$

is therefore θ independent at order m, its first θ-dependent contribution being of the order of m^2. In general the first θ-dependent contribution to the expansion of the scalar condensate in powers of the quark mass m is of the order of m^{N_f-1} and, therefore, of the order of m^{N_f} in the expansion of the vacuum energy density, analogous to Eq. (33). This is the reason why the generalization of Eq. (41) to N_f flavors reads now as follows:

$$m\left(\left\langle\sum_{f,x} S_f(x)\right\rangle_{Q=1} - \left\langle\sum_{f,x} S_f(x)\right\rangle_{Q=0}\right) = N_f + O(m). \tag{44}$$

V. SUMMARY AND CONCLUSIONS

The axion mass, an essential ingredient in the calculation of the axion abundance in the Universe, is related in the QCD axion model with the topological susceptibility χ_T at $\theta = 0$. The temperature dependence of the topological susceptibility is, therefore, just that of the axion mass.

Three papers reporting numerical results for the temperature dependence of the topological susceptibility in unquenched QCD have been recently published [13–15], and their conclusions seem not to be in agreement with each other, reflecting the high level of difficulty in measuring the topological susceptibility in the high-temperature regime.

In this paper we have shown that an analysis of some of the numerical results reported in [15] concerning the mean value of the chiral condensate at fixed topological charge suggests that the vacuum energy density is θ independent at high temperatures, but surprisingly not too high $(T \sim 2T_c)$; this result would imply a vanishing topological susceptibility and the absence of all physical effects of the $U(1)$ axial anomaly at these temperatures. More precisely, we have shown that the results of the numerical simulations of QCD at $T > T_c$ in [15,36] are in contradiction with the results of the large-volume expansion around the saddle point [(29) and (30)], but in very good agreement with the analytical perturbative expansion of the chiral condensate given by Eq. (44).

The only reason for the failure of the saddle-point expansion is that the main ingredient of this expansion, the nontrivial θ dependence of the vacuum energy density $E(\beta, m_f, \theta)$, does not work. Other intermediate solutions, like a vacuum energy density with nontrivial θ dependence for $|\theta| \leq \theta_c$, which becomes θ independent at $|\theta| > \theta_c$, would imply the existence of a phase transition at (T, θ_c); such a situation seems to be ruled out if $T \geq T_c$, at least in the pure gauge model, by the results of [9,37], which show that the critical temperature of the deconfinement phase transition decreases with θ. Therefore a θ-independent vacuum energy density seems the most plausible explanation for the failure of the saddle-point expansion.

In Sec. IV we have made a general assumption concerning the high-temperature phase of QCD, where the $SU(N_f)_A$ symmetry is restored. Basically we assume that in this phase all correlation lengths are finite in physical units, no symmetry is spontaneously broken, the model is free from infrared divergences, and the perturbative expansion of the chiral condensate in powers of the quark mass converges. A finite spatial lattice volume of linear size much larger than the inverse mass gap should be enough to reproduce the correct physical results, and, in contrast to what happens in the low-temperature broken phase, the infinite-volume limit and the chiral limit should commute. Under this assumption, we have shown that all effects of the axial anomaly should disappear in the high-temperature phase of QCD, where the $SU(N_f)_A$ symmetry is restored. The topological susceptibility and all the θ derivatives of the vacuum energy density should vanish and the theory should become θ independent at any $T > T_c$.

Incidentally, the commutativity of the chiral and infinite-volume limits is implicitly assumed by the authors of Ref. [15], since their calculations in the high-temperature regime are based on the assumption that the topological susceptibility, χ_T, can be computed in this phase from the relation $V\chi_T = \frac{2Z_1}{Z_0}$, which is the result that follows from the dilute instanton gas approximation in the $V\chi_T \ll 1$ limit.

An analysis of the physical implications of these results on the axion cosmology seems, therefore, worthwhile.

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