QCD with two flavors of Wilson fermions: The QCD vacuum, the Aoki vacuum, and other vacua

V. Azcoiti,[1] G. Di Carlo,[2] and A. Vaquero[1]

[1]*Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, Cl. Pedro Cerbuna 12, E-50009 Zaragoza, Spain*
[2]*INFN, Laboratori Nazionali del Gran Sasso, I-67010 Assergi, L'Aquila, Italy*

We discuss the vacuum structure of QCD with two flavors of Wilson fermions. We derive two possible scenarios: (i) If the spectral density $\rho_U(\lambda, \kappa)$ of the overlap Hamiltonian in a fixed background gauge field is not symmetric in λ, Hermiticity is violated and Hermiticity violation effects could influence numerical determinations of the η meson mass if we are not near enough to the continuum limit, where Hermiticity should be recovered; (ii) otherwise we argue that, under certain assumptions, new phases appear beside the Aoki phase, which can be characterized by a nonvanishing vacuum expectation value of $i\bar{\psi}_u\gamma_5\psi_u + i\bar{\psi}_d\gamma_5\psi_d$, and with vacuum states that cannot be connected with the Aoki vacua by parity-flavor symmetry transformations. Quenched numerical simulations suggest that the second scenario is more likely realized.

I. INTRODUCTION

Since the first numerical investigations of four-dimensional nonabelian gauge theories with dynamical Wilson fermions were performed in the early 80's [1,2], the understanding of the phase and vacuum structure of lattice QCD with Wilson fermions at nonzero lattice spacing, and of the way in which chiral symmetry is recovered in the continuum limit, has been a goal of lattice field theorists. The complexity of the phase structure of this model was known a long time ago. The existence of a phase with parity and flavor-symmetry breaking was conjectured for this model by Aoki in the middle 80's [3,4]. From that time on, much work has been done in order to confirm this conjecture, to establish a quantitative phase diagram for lattice QCD with Wilson fermions, and to delimit the parameters region where numerical calculations of physical quantities should be performed. References [3–20] are a representative but incomplete list of the work done on this subject.

In this paper we analyze the vacuum structure of lattice QCD with Wilson fermions at nonzero lattice spacing, with the help of the probability distribution function of the parity-flavor fermion bilinear order parameters [21,22]. We find that if the spectral density $\rho_U(\lambda, \kappa)$ of the overlap Hamiltonian, or Hermitian Dirac-Wilson operator, in a fixed background gauge field U is not symmetric in λ in the thermodynamical limit for the relevant gauge configurations, Hermiticity of $i\bar{\psi}_u\gamma_5\psi_u + i\bar{\psi}_d\gamma_5\psi_d$ will be violated at finite β. Assuming that the Aoki phase ends at finite β, this would imply the lost of any physical interpretation of this phase in terms of particle excitations. In addition, the lost of Hermiticity of $i\bar{\psi}_u\gamma_5\psi_u + i\bar{\psi}_d\gamma_5\psi_d$ at finite β also suggests that a reliable determination of the η mass would require to be near enough the continuum limit. If on the contrary the spectral density $\rho_U(\lambda, \kappa)$ of the Hermitian Dirac-Wilson operator in a fixed background

gauge field U, is symmetric in λ, we explain how, under certain assumptions, the existence of the Aoki phase implies also the appearance of other phases, in the same parameters region, which can be characterized by a nonvanishing vacuum expectation value of $i\bar{\psi}_u\gamma_5\psi_u + i\bar{\psi}_d\gamma_5\psi_d$, and with vacuum states that can not be connected with the Aoki vacua by parity-flavor symmetry transformations.

The outline of this paper is as follows. In Sec. II we derive the *p.d.f.* of $i\bar{\psi}\gamma_5\tau_3\psi$ and $i\bar{\psi}\gamma_5\psi$ and analyze the conditions to have an Aoki phase with spontaneous parity-flavor symmetry breaking. Section III contains our derivation of the *p.d.f.* of the same fermion bilinears of Sec. II but in presence of a twisted mass term in the action. We discuss also in this section how if the spectral density $\rho_U(\lambda, \kappa)$ of the Hermitian Dirac-Wilson operator in a fixed background gauge field U is not symmetric in λ, a violation of Hermiticity manifests in a negative vacuum expectation value for the square of the Hermitian operator $i\bar{\psi}\gamma_5\psi$ in the infinite lattice limit. In Sec. IV we discuss the other possible scenario i.e., we assume a symmetric spectral density $\rho_U(\lambda, \kappa)$ and then derive, assuming that the Aoki vacuum does exists, that new vacuum states should appear. These new vacua, which are not connected with the Aoki vacua by parity-flavor symmetry transformations, are analyzed in Sec. V. Section IV contains some numerical results obtained by diagonalizing quenched configurations in 4^4, 6^4, 8^4 lattices. The goal of this analysis was to distinguish between the two possible scenarios. Section VII contains our conclusions.

II. THE PROBABILITY DISTRIBUTION FUNCTION IN THE GIBBS STATE

The model we are interested in is QCD with two degenerate Wilson quarks. The fermionic part of the Euclidean action is
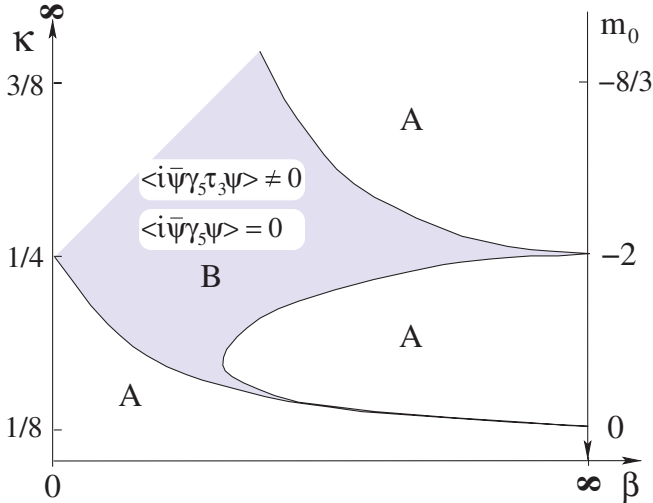
FIG. 1 (color online).   Aoki (B) and physical (A) region in the (β, κ) plane. Adapted from [16] with courtesy of the authors.

$$S_F = \bar{\psi} W(\kappa) \psi, \tag{1}$$

where $W(\kappa)$ is the Dirac-Wilson operator, κ is the hopping parameter, which is related to the bare fermion mass m_0 by $\kappa = 1/(8 + 2m_0)$, and flavor indices are implicit ($W(\kappa)$ is a two-block diagonal matrix). The standard wisdom on the phase diagram of this model in the gauge coupling β, κ plane is the one shown in Fig. 1. The two different regions observed in this phase diagram, A and B, can be characterized as follows; in region A parity and flavor symmetries are realized in the vacuum, which is supposed to be unique. The Gibbs state is then very simple in this region, and continuum QCD should be obtained by taking the $g^2 \to 0$, $\kappa \to 1/8$ limit from within region A. We will call region A the QCD region. In region B, on the contrary, parity and flavor symmetries are spontaneously broken, there are many degenerate vacua connected by parity-flavor transformations in this region, and the Gibbs state is therefore made up from many equilibrium states. In what follows we will call region B as the Aoki region.

The order parameters to distinguish the Aoki region from the QCD region are $i\bar{\psi}\gamma_5\tau_j\psi$ and $i\bar{\psi}\gamma_5\psi$, with τ_j the three Pauli matrices. For the more standard election, $j = 3$, they can be written in function of the up and down quark fields as follows

$$\begin{aligned} i\bar{\psi}\gamma_5\tau_3\psi &= i\bar{\psi}_u\gamma_5\psi_u - i\bar{\psi}_d\gamma_5\psi_d \\ i\bar{\psi}\gamma_5\psi &= i\bar{\psi}_u\gamma_5\psi_u + i\bar{\psi}_d\gamma_5\psi_d. \end{aligned} \tag{2}$$

The Aoki phases are characterized by [4]

$$\langle i\bar{\psi}\gamma_5\tau_3\psi \rangle \neq 0 \qquad \langle i\bar{\psi}\gamma_5\psi \rangle = 0. \tag{3}$$

The first of the two condensates breaks both parity and flavor symmetries. The nonvanishing vacuum expectation value of this condensate signals the spontaneous breaking of the $SU(2)$ flavor symmetry down to $U(1)$, with two Goldstone pions. Notwithstanding parity is spontaneously broken if the first equation in (3) holds, the vacuum expectation value of the flavor diagonal condensate $\langle i\bar{\psi}\gamma_5\psi \rangle$ vanishes because it is also order parameter for a discrete symmetry, composition of parity and discrete flavor rotations, which is assumed to be realized [4].

Following the lines developed in [21], we wish to write the *p.d.f.* of the two fermion bilinear order parameters (2). The motivation to develop this formalism was precisely the study of the vacuum invariance (noninvariance), in quantum theories regularized on a space time lattice, under symmetry transformations which, as chiral, flavor or baryon symmetries, involve fermion fields. Notwithstanding that Grassmann variables cannot be simulated in a computer, it was shown in [21] that an analysis of spontaneous symmetry breaking based on the use of the *p.d.f.* of fermion local operators can also be done in *QFT* with fermion degrees of freedom. The starting point is to choose an order parameter for the desired symmetry $O(\psi, \bar{\psi})$ (typically a fermion bilinear) and characterize each vacuum state α by the expectation value c_α of the order parameter in the α state

$$c_\alpha = \frac{1}{V} \int \langle O(x) \rangle_\alpha d^4x. \tag{4}$$

The *p.d.f.* $P(c)$ of the order parameter will be given by

$$P(c) = \sum_\alpha w_\alpha \delta(c - c_\alpha), \tag{5}$$

which can also be written as [21]

$$P(c) = \left\langle \delta\left(\frac{1}{V} \int O(x) d^4x - c\right) \right\rangle, \tag{6}$$

the mean value computed with the integration measure of the path integral formulation of the Quantum Theory.

The Fourier transform $P(q) = \int e^{iqc} P(c) dc$ can be written, for the model we are interested in, as

$$P(q) = \frac{\int [dU][d\bar{\psi}d\psi] \exp\{-S_{\text{YM}} + \bar{\psi}W(\kappa)\psi + \frac{iq}{V}\int d^4x O(x)\}}{\int [dU][d\bar{\psi}d\psi] \exp\{-S_{\text{YM}} + \bar{\psi}W(\kappa)\psi\}}. \tag{7}$$

In the particular case in which O is a fermion bilinear of $\bar{\psi}$ and ψ

$$O(x) = \bar{\psi}(x)\tilde{O}\psi(x) \tag{8}$$

with $\tilde{O}$ any matrix with Dirac, color and flavor indices, Eq. (7) becomes

$$P(q) = \frac{\int[dU][d\bar{\psi}d\psi]\exp\{-S_{YM} + \bar{\psi}(W(\kappa) + \frac{iq}{V}\tilde{O})\psi\}}{\int[dU][d\bar{\psi}d\psi]\exp\{-S_{YM} + \bar{\psi}W(\kappa)\psi\}}. \tag{9}$$

Integrating out the fermion fields in (9) one gets

$$P(q) = \frac{\int[dU]e^{-S_{YM}}\det(W(\kappa) + \frac{iq}{V}\tilde{O})}{\int[dU]e^{-S_{YM}}\det W(\kappa)}, \tag{10}$$

which can also be expressed as the following mean value

$$P(q) = \left\langle\frac{\det(W(\kappa) + \frac{iq}{V}\tilde{O})}{\det W(\kappa)}\right\rangle, \tag{11}$$

computed in the effective gauge theory with the integration measure

$$[dU]e^{-S_{YM}}\det W(\kappa).$$

Notice that zero modes of the Dirac-Wilson operator, which would produce a singularity of the operator in (11), are suppressed by the fermion determinant in the integration measure (zero mode configurations have on the other hand vanishing measure).

The particular form expected for the *p.d.f.* $P(c)$, $P(q)$, depends on the realization of the corresponding symmetry in the vacuum. A symmetric vacuum will give

$$P(c) = \delta(c) \qquad P(q) = 1, \tag{12}$$

whereas, if we have for instance a $U(1)$ symmetry which is spontaneously broken, the expected values for $P(c)$ and $P(q)$ are [21]

$$P(c) = [\pi(c_0^2 - c^2)^{1/2}]^{-1} \qquad -c_0 < c < c_0,$$
$$\text{otherwise} \qquad P(c) = 0,$$
$$P(q) = \frac{1}{2\pi}\int_{-\pi}^{\pi}d\theta e^{iqc_0\cos\theta}, \tag{13}$$

the last being the well known zeroth order Bessel function of the first kind, $J_0(qc_0)$.

In the simpler case in which a discrete $Z(2)$ symmetry is spontaneously broken, the expected form is

$$P(c) = \frac{1}{2}\delta(c - c_0) + \frac{1}{2}\delta(c + c_0) \qquad P(q) = \cos(qc_0) \tag{14}$$

or a sum of symmetric delta functions ($P(c)$) and a sum of cosines ($P(q)$) if there is an extra vacuum degeneracy.

If we call $P_j(q)$, $P_0(q)$ the *p.d.f.* of $i\bar{\psi}\gamma_5\tau_j\psi$ and $i\bar{\psi}\gamma_5\psi$ in momentum space, we have

$$P_1(q) = P_2(q) = P_3(q) = \left\langle\prod_j\left(-\frac{q^2}{V^2\lambda_j^2} + 1\right)\right\rangle$$
$$P_0(q) = \left\langle\prod_j\left(\frac{q}{V\lambda_j} + 1\right)^2\right\rangle, \tag{15}$$

where V is the number of degrees of freedom (including color and Dirac but not flavor d.o.f.) and λ_j are the real eigenvalues of the Hermitian Dirac-Wilson operator $\bar{W}(\kappa) = \gamma_5 W(\kappa)$. Notice that whereas $P_3(q)$ has not a definite sign, $P_0(q)$ is always positive definite.

The q derivatives of $P(q)$ give us the moments of the distribution $P(c)$. In particular we have

$$\frac{d^n P(q)}{dq^n}\bigg|_{q=0} = i^n\langle c^n\rangle. \tag{16}$$

Since c is order parameter for the symmetries of the lattice action and we integrate over all the Gibbs state, the first moment will vanish always, independently of the realization of the symmetries. The first nonvanishing moment, if the symmetry is spontaneously broken, will be the second. Thus, for the particular case

$$c_0 = \frac{1}{V}\sum_x i\bar{\psi}(x)\gamma_5\psi(x) \qquad c_3 = \frac{1}{V}\sum_x i\bar{\psi}(x)\gamma_5\tau_3\psi(x), \tag{17}$$

we get

$$\langle c_0^2\rangle = 2\left\langle\frac{1}{V^2}\sum_j\frac{1}{\lambda_j^2}\right\rangle - 4\left\langle\left(\frac{1}{V}\sum_j\frac{1}{\lambda_j}\right)^2\right\rangle$$
$$\langle c_3^2\rangle = 2\left\langle\frac{1}{V^2}\sum_j\frac{1}{\lambda_j^2}\right\rangle. \tag{18}$$

In the QCD region flavor symmetry is realized. The *p.d.f.* of c_3 will be then $\delta(c_3)$ and $\langle c_3^2\rangle = 0$. We get then

$$\langle c_0^2\rangle = -4\left\langle\left(\frac{1}{V}\sum_j\frac{1}{\lambda_j}\right)^2\right\rangle,$$

which should vanish since parity is also realized in this region. Furthermore a negative value of $\langle c_0^2\rangle$ would violate Hermiticity of $i\bar{\psi}\gamma_5\psi$. We will come back to this point in the next section.

In the Aoki region [4] there are vacuum states in which the condensate c_3 (17) takes a nonvanishing vacuum expectation value. This implies that the *p.d.f.* $P(c_3)$ will not be $\delta(c_3)$ and therefore $\langle c_3^2\rangle$ (18) will not vanish. Indeed expression (18) for $\langle c_3^2\rangle$ seems to be consistent with the Banks and Casher formula [23] which relates the spectral density of the Hermitian Dirac-Wilson operator at the origin with the vacuum expectation value of c_3 [10].

If, on the other hand, $\langle i\bar{\psi}\gamma_5\psi\rangle = 0$ in one of the Aoki vacua, as conjectured in [4], $\langle i\bar{\psi}\gamma_5\psi\rangle = 0$ in all the other vacua which are connected with the standard Aoki vacuum by a parity-flavor transformation, since $i\bar{\psi}\gamma_5\psi$ is invariant

under flavor transformations and change sign under parity. Therefore if we assume that these are all the degenerate vacua, we conclude that $P(c_0) = \delta(c_0)$ and $\langle c_0^2 \rangle = 0$, which would imply the following nontrivial relation

$$\left\langle \frac{1}{V^2} \sum_j \frac{1}{\lambda_j^2} \right\rangle = 2 \left\langle \left(\frac{1}{V} \sum_j \frac{1}{\lambda_j} \right)^2 \right\rangle \neq 0. \qquad (19)$$

III. QCD WITH A TWISTED MASS TERM: THE NONSYMMETRIC CASE

In this section we will consider lattice QCD with Wilson fermions with the standard action of previous section, plus a source term

$$\sum_x i m_t \bar{\psi}(x) \gamma_5 \tau_3 \bar{\psi}(x) \qquad (20)$$

that explicitly breaks flavor and parity. The flavor symmetry is thus broken from $SU(2)$ to $U(1)$. This is the standard way to analyze spontaneous symmetry breaking. First one takes the thermodynamic limit and then the vanishing source term limit.

We can calculate again the p.d.f. $\bar{P}_0(q)$ and $\bar{P}_3(q)$ of $i\bar{\psi}\gamma_5\psi$ and $i\bar{\psi}\gamma_5\tau_3\psi$ with this modified action. Simple algebra give us the following expressions

$$\bar{P}_0(q) = \left\langle \prod_j \left(\frac{\frac{q^2}{V^2} + \frac{2q}{V}\lambda_j}{m_t^2 + \lambda_j^2} + 1 \right) \right\rangle$$
$$\qquad (21)$$
$$\bar{P}_3(q) = \left\langle \prod_j \left(\frac{\frac{q^2}{V^2} + \frac{2q}{V}im_t}{m_t^2 + \lambda_j^2} - 1 \right) \right\rangle,$$

where again λ_j are the real eigenvalues of the Hermitian Dirac-Wilson operator and the mean values are computed now with the integration measure of the lattice QCD action modified with the symmetry breaking source term.

By taking the q derivatives at the origin of $\bar{P}_0(q)$ and $\bar{P}_3(q)$ we obtain

$$\langle c_0 \rangle = \frac{2i}{V} \left\langle \sum_j \frac{\lambda_j}{m_t^2 + \lambda_j^2} \right\rangle$$

$$\langle c_0^2 \rangle = \frac{4}{V^2} \left\langle \sum_j \frac{\lambda_j^2}{(m_t^2 + \lambda_j^2)^2} \right\rangle - \frac{2}{V^2} \left\langle \sum_j \frac{1}{m_t^2 + \lambda_j^2} \right\rangle \quad (22)$$
$$\qquad - 4 \left\langle \left(\frac{1}{V} \sum_j \frac{\lambda_j}{m_t^2 + \lambda_j^2} \right)^2 \right\rangle$$

and

$$\langle c_3 \rangle = \frac{2}{V} m \left\langle \sum_j \frac{1}{m_t^2 + \lambda_j^2} \right\rangle. \qquad (23)$$

Equation (23) is well known. If we take the infinite volume limit and then the $m \to 0$ limit we get the Banks and Casher result

$$\langle c_3 \rangle = 2\pi\rho(0) \qquad (24)$$

which relates a nonvanishing spectral mean density of the Hermitian Wilson operator at the origin with the spontaneous breaking of parity and flavor symmetries.

The first equation in (22) is actually unpleasant since it predicts an imaginary number for the vacuum expectation value of a Hermitian operator. However it is easy to see that $\langle c_0 \rangle = 0$ because it is order parameter for a symmetry of the modified lattice action, the composition of parity with discrete flavor rotations around the x or y axis.

Concerning the second equation in (22), one can see that the first and second contributions to $\langle c_0^2 \rangle$ vanish in the infinite volume limit for every nonvanishing value of m. The third contribution however, which is negative, will vanish only if the spectral density of eigenvalues of the Hermitian Wilson operator $\rho_U(\lambda)$ for any background gauge field U is an even function of λ. This is actually not true at finite values of V, and some authors [8,10] suggest that the symmetry of the eigenvalues will be recovered not in the thermodynamic limit, but only in the zero lattice spacing or continuum limit. If we take this last statement as true, we should conclude:
  (i) The Aoki phase, which seems not to be connected with the critical continuum limit point ($g^2 = 0$, $\kappa = 1/8$) [16,17] is unphysical since the $\langle c_0^2 \rangle$ would be negative in this phase and this result breaks Hermiticity.
  (ii) In the standard QCD phase, where parity and flavor symmetries are realized in the vacuum, we should have however negative values for the vacuum expectation value of the square of the Hermitian operator $i\bar{\psi}\gamma_5\psi$, except very near to the continuum limit. Since this operator is related to the η meson, one can expect in such a case important finite lattice spacing effects in the numerical determinations of the η-meson mass.

This is the first of the two possible scenarios mentioned in the first section of this article. In the next section we will assume a symmetric spectral density of eigenvalues of the Hermitian Wilson operator $\rho_U(\lambda)$ for any background gauge field U in the thermodynamic limit, and will derive the second scenario.

IV. QCD WITH A TWISTED MASS TERM: SYMMETRIC SPECTRAL DENSITY OF EIGENVALUES

In this section we will assume that the spectral density of eigenvalues of the Hermitian Wilson operator $\rho_U(\lambda)$ for any background gauge field U is an even function of λ. In such a case Eq. (22) will give a vanishing value for $\langle c_0^2 \rangle$ at any value of m_t

$$\langle c_0^2 \rangle = 0. \qquad (25)$$

Therefore the p.d.f. of c_0 is $\delta(c_0)$ and

$$\langle i\bar{\psi}\gamma_5\psi\rangle = 0 \qquad (26)$$

for any value of m_t, and also in the $m_t \rightarrow 0$ limit. Thus we can confirm that under the assumed condition, $\langle i\bar{\psi}\gamma_5\psi\rangle = 0$ in the Aoki vacuum selected by the external source (20), as stated in [4]; but since $i\bar{\psi}\gamma_5\psi$ is flavor invariant and change sign under parity, we can conclude that $\langle i\bar{\psi}\gamma_5\psi\rangle = 0$, not only in the vacuum selected by the external source (20), but also in all the Aoki vacua which can be obtained from the previous one by parity-flavor transformations. In order to see the fact that, if there is an Aoki phase with parity-flavor symmetry spontaneously broken, the previous vacua are not all the possible vacua, we will assume that is false and will get a contradiction.

If all the vacua are the one selected by the twisted mass term and those obtained from it by parity-flavor transformations, the spectral density of the Hermitian Wilson operator will be always an even function of λ, since the eigenvalues of this operator change sign under parity and are invariant under flavor transformations. Then the symmetry of $\rho_U(\lambda)$ will be realized also at $m_t = 0$ in the Gibbs state. Now let us come back to expression (18) which give us the vacuum expectation values of the square of $i\bar{\psi}\gamma_5\psi$ and $i\bar{\psi}\gamma_5\tau_3\psi$ as a function of the spectrum of the Hermitian Wilson operator, but averaged over all the Gibbs state (without the external symmetry breaking source (20)). By subtracting the two equations in (18) we get

$$\langle c_3^2\rangle - \langle c_0^2\rangle = 4\left\langle\left(\frac{1}{V}\sum_j\frac{1}{\lambda_j}\right)^2\right\rangle. \qquad (27)$$

This equation would *naively* vanish, if the spectral density of eigenvalues of the Hermitian Wilson operator were an even function of λ. Therefore we would reach the following conclusion for the Gibbs state

$$\langle c_3^2\rangle = \langle c_0^2\rangle. \qquad (28)$$

Nevertheless, S. Sharpe put into evidence in a private communication (developed deeply in [24]) an aspect that we, somewhat, overlooked: A subleading contribution to the spectral density may affect (28) in the Gibbs state (ϵ-regime, in χPT terminology), in such a way that, not only $\langle c_0^2\rangle$, but every even moment of $i\bar{\psi}\gamma_5\psi$ would vanish, restoring the standard Aoki picture. The thesis of Sharpe, although possible, would enforce an infinite series of *sum rules* to be complied, similar to those found by Leutwyler and Smilga in the continuum [25]. We agree that such a possibility is open, at least from a purely mathematical point of view: In fact subleading contributions to the spectral density may exist, and conspire to enforce the vanishing of all the even moments of the *p.d.f.* of $i\bar{\psi}\gamma_5\psi$. However we believe such possibility not to be very realistic, and indeed we have physical arguments, which will be the basis for subsequent work on the topic, suggesting that the Aoki scenario is incomplete. Therefore,

we will reasonably assume in the following (28) to be true, in the case of a symmetric $\rho_U(\lambda)$, assumption that leads us to the conclusion that the *Chiral Perturbation Theory may be incomplete*, for the new vacua derived from (28) are not predicted in χPT.

If as conjectured by Aoki and verified by numerical simulations, a phase with a nonvanishing vacuum expectation value of $i\bar{\psi}\gamma_5\tau_3\psi$ does exists, the mean value in the Gibbs state $\langle c_3^2\rangle$ inside this phase will be nonzero. Then Eq. (28) tell us that also $\langle c_0^2\rangle$ will be nonzero inside this phase. But since in the Aoki vacua $\langle c_0^2\rangle = 0$, this is in contradiction with the assumption that the Aoki vacua are all possible vacua. This is the second possible scenario mentioned in the Introduction of this article.

V. THE NEW VACUA

To understand the physical properties of these new vacuum states we will assume, inspired by the numerical results reported in the next section, that the spectral density of eigenvalues $\rho_U(\lambda)$ is an even function of λ in the Gibbs state of the Aoki region ($m_t = 0$). Then Eq. (28) holds (taking into account the aforementioned discussion raised by S. Sharpe), and hence the *p.d.f.* of the flavor singlet $i\bar{\psi}\gamma_5\psi$ order parameter can not be $\delta(c_0)$ inside the Aoki phase, and therefore new vacuum states characterized by a nonvanishing vacuum expectation value of $i\bar{\psi}\gamma_5\psi$ should appear. These new vacua can not be connected, by mean of parity-flavor transformations, to the Aoki vacua, as previously discussed.

In order to better characterize these new vacua, we have added to the lattice QCD action the source term

$$im_t\bar{\psi}\gamma_5\tau_3\psi + i\theta\bar{\psi}\gamma_5\psi, \qquad (29)$$

which breaks more symmetries than (20), but still preserves the $U(1)$ subgroup of the $SU(2)$ flavor. By computing again the first moment of the *p.d.f.* of $i\bar{\psi}\gamma_5\psi$ and $i\bar{\psi}\gamma_5\tau_3\psi$ and taking into account that the mean value of the first of these operators is an odd function of θ whereas the second one is an even function of θ, we get

$$\langle i\bar{\psi}\gamma_5\psi\rangle = -\frac{2\theta}{V}\left\langle\sum_j\frac{-\lambda_j^2 + m_t^2 - \theta^2}{(\lambda_j^2 + m_t^2 - \theta^2)^2 + 4\theta^2\lambda_j^2}\right\rangle$$

$$\langle i\bar{\psi}\gamma_5\tau_3\psi\rangle = \frac{2m_t}{V}\left\langle\sum_j\frac{\lambda_j^2 + m_t^2 - \theta^2}{(\lambda_j^2 + m_t^2 - \theta^2)^2 + 4\theta^2\lambda_j^2}\right\rangle, \qquad (30)$$

where λ_j are again the eigenvalues of the Hermitian Wilson operator and the mean values are computed using the full integration measure of lattice QCD with the extra external source (29). This integration measure is not positive definite due to the presence of the $i\bar{\psi}\gamma_5\psi$ term in the action.

By choosing $\theta = rm_t$ in the action and taking the thermodynamic limit we get for the two order parameters the following expressions

$$\langle i\bar{\psi}\gamma_5\psi\rangle = \int \frac{2rm_t\lambda^2 - 2rm_t^3(1-r^2)}{(m_t^2(1-r^2)+\lambda^2)^2 + 4r^2m_t^2\lambda^2}\rho(\lambda)d\lambda$$

$$\left\langle i\bar{\psi}\gamma_5\tau_3\psi\right\rangle = \int \frac{2m_t^3(1-r^2) + 2m_t\lambda^2}{(m_t^2(1-r^2)+\lambda^2)^2 + 4r^2m_t^2\lambda^2}\rho(\lambda)d\lambda,$$

$$(31)$$

where $\rho(\lambda)$ is the mean spectral density of the Hermitian Wilson operator averaged with the full integration measure.

Taking now the $m_t \to 0$ limit i.e., approaching the vanishing external source (29) point in the θ, m_t plane on a line crossing the origin and with slope r, we obtain

$$\langle i\bar{\psi}\gamma_5\psi\rangle = 2\rho(0)\int_{-\infty}^{+\infty} \frac{rt^2 - r(1-r^2)}{(1-r^2+t^2)^2 + 4r^2t^2}dt$$

$$\langle i\bar{\psi}\gamma_5\tau_3\psi\rangle = 2\rho(0)\int_{-\infty}^{+\infty} \frac{1-r^2+t^2}{(1-r^2+t^2)^2 + 4r^2t^2}dt.$$

$$(32)$$

In the particular case of $r = 0$ ($\theta = 0$) we get the Banks and Casher formula

$$\langle i\bar{\psi}\gamma_5\tau_3\psi\rangle = 2\pi\rho(0). \qquad (33)$$

We see how, if $\rho(0)$ does not vanish, we can get many vacua characterized by a nonvanishing value of the two order parameters $i\bar{\psi}\gamma_5\psi$ and $i\bar{\psi}\gamma_5\tau_3\psi$. We should point out that the value of $\rho(0)$ could depend on the slope r of the straight line along which we approach the origin in the θ, m plane, and therefore, even if results of numerical simulations suggest that $\rho(0) \neq 0$ when we approach the origin along the line of vanishing slope, this does not guarantee that the same holds for other slopes. However the discussion in the first half of this section tell us that if $\rho(0) \neq 0$ at $r = 0$, $\rho(0)$ should be nonvanishing for other values of r.

VI. QUENCHED NUMERICAL SIMULATIONS

In order to distinguish what of the two possible scenarios derived in the previous sections is realized, we have performed quenched simulations of lattice QCD with Wilson fermions in 4^4, 6^4 and 8^4 lattices. We have generated an ensemble of well uncorrelated configurations for each volume and then a complete diagonalization of the Hermitian Wilson matrix, for each configuration, gives us the respective eigenvalues. We measured the volume dependence of the asymmetries in the eigenvalue distribution of the Hermitian Wilson operator, both inside and outside the Aoki phase.

We want to notice that because of kinematic reasons (properties of the Dirac matrices), the trace of all odd p-powers of the Hermitian Wilson operator $\bar{W}(\kappa) = \gamma_5 W(\kappa)$ vanish until $p = 7$, this included. This means that the asymmetries in the eigenvalue distribution of $\bar{W}(\kappa)$ start to manifest with a nonvanishing value of the ninth moment of the distribution. We have found that these asymmetries,
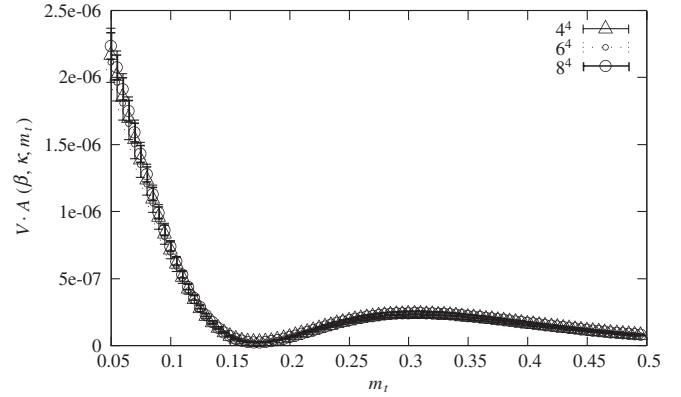

FIG. 2. Point outside of the Aoki phase ($\beta = 0.001$, $\kappa = 0.17$) and in the strong coupling regime. The superposition of plots clearly states that the asymmetry of the eigenvalue distribution decreases as $\frac{1}{V}$. Statistics: 240 configurations (4^4), 2998 conf. (6^4) and 806 conf. (8^4).

even if small, are clearly visible in the numerical simulations.

In Figs. from 2–6 we plot the quenched mean value

$$A(\beta, \kappa, m_t) = \left\langle \left(\frac{1}{V}\sum_j \frac{\lambda_j}{m_t^2 + \lambda_j^2}\right)^2\right\rangle_Q \qquad (34)$$

multiplied by the volume for three different volumes, in order to see the scaling of the asymmetries in the eigenvalue distribution of $\bar{W}(\kappa)$. As previously discussed, $A(\beta, \kappa, m_t)$ give us a quantitative measure of these asymmetries. We have added an extra V factor to make the plots for the three different volumes distinguishable. Since we found that the value of $A(\beta, \kappa, m_t)$ decreased as the volume increased, the plots of the larger volumes were negligible with respect to the plot of the smaller volume 4^4. Multiplying by V all the plots are of the same magnitude order.
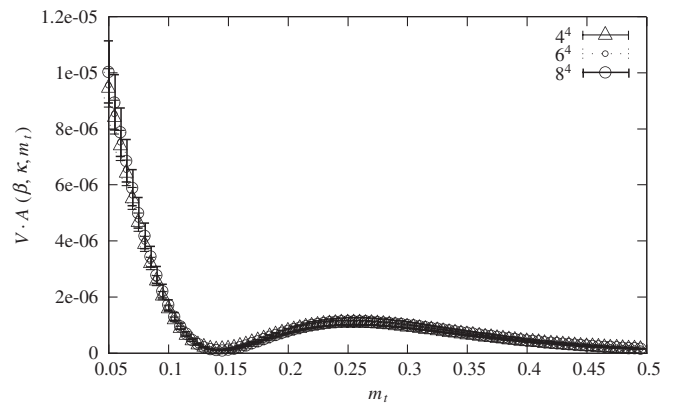

FIG. 3. Another point outside of the Aoki phase ($\beta = 5.0$, $\kappa = 0.15$) in a region in which QCD simulations are commonly performed. The conclusion is the same as in Fig. 2. Statistics: 400 conf. (4^4), 900 conf. (6^4) and 200 conf. (8^4).
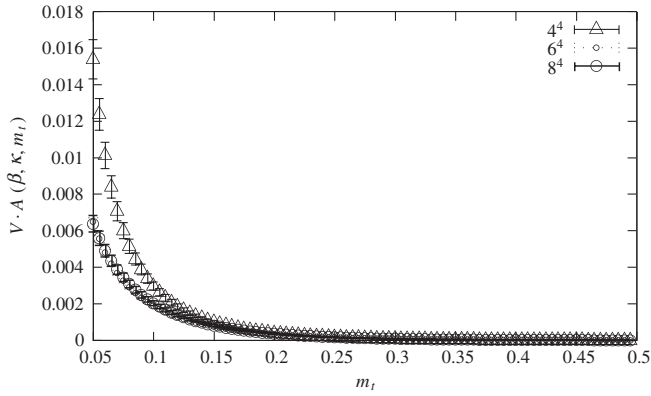
FIG. 4.   Point inside the Aoki phase ($\beta = 0.001$, $\kappa = 0.30$) and in the strong coupling regime. Although there is no clear superposition of plots, it is evident that the asymmetry goes to zero as the volume increases. Statistics: 368 conf. (4^4), 1579 conf. (6^4) and 490 conf. (8^4).

The m_t term in the denominator of (34) acts also as a regulator in the quenched approximation, where configurations with zero or near-zero modes are not suppressed by the fermion determinant. This is very likely the origin of the large fluctuations observed in the numerical measurements of (34) near $m_t = 0$ in the quenched case. That is why our plots are cut below $m_t = 0.05$; in the physical phase, this cutoff is not really needed, but in the Aoki phase it is more likely to find zero modes which spoil the distribution.

Figures 2 and 3 contain our numerical results in 4^4, 6^4 and 8^4 lattices at $\beta = 0.001$, $\kappa = 0.17$ and $\beta = 5.0$, $\kappa = 0.15$. These first two points are outside the Aoki phase, the first one in the strong coupling region. The second one intends to be a point where typically QCD simulations are performed.

Figures 4–6, represent our numerical results in 4^4, 6^4 and 8^4 lattices at $\beta = 0.001$, $\kappa = 0.30$, $\beta = 3.0$, $\kappa = 0.30$ and $\beta = 4.0$, $\kappa = 0.24$. These points are well inside the Aoki
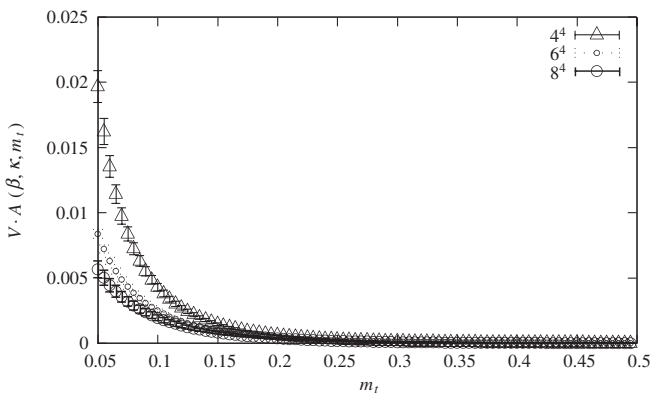

FIG. 5.   Point inside the Aoki phase ($\beta = 3.0$, $\kappa = 0.30$). The asymmetry disappears as the volume increases. Statistics: 400 conf. (4^4), 1174 conf. (6^4) and 107 conf. (8^4).
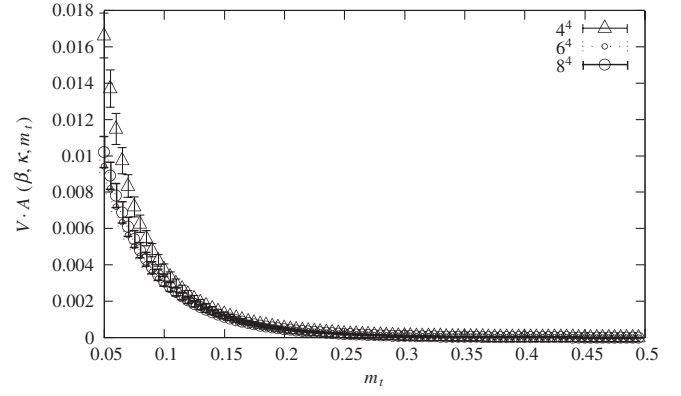

FIG. 6.   Point inside the Aoki phase ($\beta = 4.0$, $\kappa = 0.24$). Same conclusions as in the other Aoki plots. Statistics: 398 conf. (4^4), 1539 conf. (6^4) and 247 conf. (8^4).

phase, and the structure of the distribution is different from the structure observed in the previous plots of the physical phase. Nevertheless, the qualitative behavior as the volume increases is the same.

We observe large fluctuations in the plotted quantity near $m_t = 0$, specially inside the Aoki phase. However the behavior with the lattice volume may suggests a vanishing value of $A(\beta, \kappa, m_t)$ in the infinite volume limit in both regions, inside and outside the Aoki phase. If this is actually the case in the unquenched model, the second scenario discussed in this article would eventually be realized.

VII. CONCLUSIONS

We have analyzed the vacuum structure of lattice QCD with two degenerate Wilson flavors at nonzero lattice spacing, with the help of the probability distribution function of the parity-flavor fermion bilinear order parameters. From this analysis two possible scenarios emerge.

In the first scenario we assume a spectral density $\rho_U(\lambda, \kappa)$ of the Hermitian Dirac-Wilson operator, in a fixed background gauge field U, not symmetric in λ. This property is realized at finite V for the single gauge configurations, even if a symmetric distribution of eigenvalues is recovered if we average over parity conjugate configurations. We find that under such an assumption, Hermiticity of $i\bar{\psi}_u\gamma_5\psi_u + i\bar{\psi}_d\gamma_5\psi_d$ will be violated at finite β. This lost of Hermiticity for the pseudoscalar flavor singlet operator suggests that a reliable determination of the η mass would require to be near enough the continuum limit where the symmetry of the spectral density $\rho_U(\lambda, \kappa)$ should be recovered. Furthermore assuming that the Aoki phase ends at finite β, the violation of Hermiticity obtained in this scenario implies the lost of any physical interpretation of this phase in terms of particle excitations.

In the second scenario a symmetric spectral density $\rho_U(\lambda, \kappa)$ of the Hermitian Dirac-Wilson operator in the infinite volume limit is assumed, and then we show that the

existence of the Aoki phase implies also the appearance of other phases, in the same parameters region, which can be characterized by a nonvanishing vacuum expectation value of $i\bar{\psi}_u \gamma_5 \psi_u + i\bar{\psi}_d \gamma_5 \psi_d$, and with vacuum states that can not be connected with the Aoki vacua by parity-flavor symmetry transformations. These phases, however, are not related to those mentioned in [26], for we keep the twisted mass parameter m_5 equal to zero, whereas the phases studied by G. Münster appear at large m_5.

Sharpe and Singleton [10,13] performed an analysis of lattice QCD with two flavors of Wilson fermions near the continuum limit, by mean of the chiral effective Lagrangians. In their analysis, they found essentially two possible realizations, depending on the sign of a coefficient c_2, which appears in the potential energy, expanded up to second order in the quark mass term. If c_2 is positive, a phase with spontaneous flavor symmetry breaking and an Aoki vacuum can be identified. If, on the contrary, $c_2 < 0$, flavor symmetry is realized in the vacuum and a first order transition should appear. Either case may be realized in different regions of parameter space. Indeed numerical simulations with dynamical fermions, performed at small lattice spacing [27], give evidences of metastability that can be related with the existence of a first order phase transition and hence $c_2 < 0$, while the Aoki phase found at smaller β values [16] supports $c_2 > 0$. We want to emphasize that the new vacua we find are coexisting with the standard Aoki vacuum. These new vacua do exist if, and only if, the Aoki vacuum exists. But these new vacua are not explained in any way in the chiral effective Lagrangian approximation of Sharpe and Singleton. On the other hand, in order to recover the standard Aoki picture via χPT, an infinite set of sum rules for the eigenvalues of the Hermitian Wilson operator must be imposed. As we stated previously, this possibility does not appeal us, in the sense that it seems unphysical (we would call it a ''mathematical'' possibility). Nevertheless we have not definite proof of the new vacua.

From our position, these conclusions lead us to cast a doubt into the completeness of the chiral perturbation theory. In any case we believe that, in order to definitely clarify this issue, a careful investigation of the spectral properties of Hermitian Dirac-Wilson operator for actual gauge field configuration in the full unquenched theory is mandatory.

In order to distinguish what of the two possible scenarios, as mentioned at the beginning of this section, is realized, we performed quenched simulations of lattice QCD with Wilson fermions in 4^4, 6^4 and 8^4 lattices, and measured the volume dependence of the asymmetries in the eigenvalue distribution of the Hermitian Wilson operator, both inside and outside the Aoki phase. To measure this asymmetries we diagonalized exactly the Hermitian Wilson operator for all the gauge configurations generated with the quenched measure, and measured the quenched average $A(\beta, \kappa, m)$ (34). Because of the fact that configurations with zero or near-zero modes are not suppressed by the fermion determinant in the quenched case, this quantity fluctuates violently near $m = 0$, specially for the points in the Aoki phase. Notwithstanding that, the observed behavior with the lattice volume seems to suggest a vanishing value of $A(\beta, \kappa, m)$ in the infinite volume limit, both inside and outside the Aoki phase. If this were actually the case in the unquenched model, the second scenario discussed in this article would be realized. However a verification of these results in the unquenched case would be very relevant in order to discard the first scenario.

ACKNOWLEDGMENTS

[1] V. Azcoiti and A. Nakamura, Phys. Rev. D **27**, 2559 (1983).
[2] H. W. Hamber, Nucl. Phys. **B251**, 182 (1985).
[3] S. Aoki, Phys. Rev. D **30**, 2653 (1984).
[4] S. Aoki, Phys. Rev. Lett. **57**, 3136 (1986).
[5] S. Aoki, S. Boettcher, and A. Gocksch, BNL, Report No. BNL-ABG-1, 1993.
[6] K. M. Bitar, Phys. Rev. D **56**, 2736 (1997).
[7] S. Aoki, T. Kaneda, and A. Ukawa, Phys. Rev. D **56**, 1808 (1997).
[8] K. M. Bitar, U. M. Heller, and R. Narayanan, Phys. Lett. B **418**, 167 (1998).
[9] R. G. Edwards, U. M. Heller, R. Narayanan, and R. L. Singleton, Jr, Nucl. Phys. **B518**, 319 (1998).
[10] S. R. Sharpe and R. Singleton, Jr, Phys. Rev. D **58**, 074501 (1998).
[11] S. Aoki, Nucl. Phys. B, Proc. Suppl. **60A**, 206 (1998).
[12] K. Bitar, Nucl. Phys. B, Proc. Suppl. **63A-C**, 829 (1998).
[13] S. Sharpe and R. L. Singleton, Jr, Nucl. Phys. B, Proc. Suppl. **73**, 234 (1999).
[14] R. Kenna, C. Pinto, and J. C. Sexton, Phys. Lett. B **505**, 125 (2001).
[15] M. Golterman and Y. Shamir, Phys. Rev. D **68**, 074501 (2003).

[16] E. M. Ilgenfritz, W. Kerler, M. Müller-Preussker, A. Sternbeck, and H. Stuben, Phys. Rev. D **69**, 074511 (2004).

[17] A. Sternbeck, E. M. Ilgenfritz, W. Kerler, M. Müller-Preussker, and H. Stuben, Nucl. Phys. B, Proc. Suppl. **129-130**, 898 (2004).

[18] M. Golterman, S. R. Sharpe, and R. Singleton, Jr., Nucl. Phys. B, Proc. Suppl. **140**, 335 (2005).

[19] E. M. Ilgenfritz, W. Kerler, M. Müller-Preussker, A. Sternbeck, and H. Stuben, HU-EP-05/78, ZIB-Report 05-48, SFB/CPP-05-81, 2005.

[20] VE. M. Ilgenfritz, M. Müller-Preussker, M. Petschlies, K. Jansen, M. P. Lombardo, O. Philipsen, L. Zeidlewicz, and A. Sternbeck, Proc. Sci., Lattice2007 (2008) 323.

[21] V. Azcoiti, V. Laliena, and X. Q. Luo, Phys. Lett. B **354**, 111 (1995).

[22] V. Azcoiti, G. Di Carlo, and A. Vaquero, J. High Energy Phys. 04 (2008) 035.

[23] T. Banks and A Casher, Nucl. Phys. **B169**, 103 (1980).

[24] S. Sharpe, arXiv:0811.0409

[25] H. Leutwyler and A. Smilga, Phys. Rev. D **46**, 5607 (1992).

[26] G. Münster, J. High Energy Phys. 09 (2004) 035.

[27] F. Farchioni *et al.*, Eur. Phys. J. C **39**, 421 (2005); Nucl. Phys. B, Proc. Suppl. **140**, 240 (2005); Phys. Lett. B **624**, 324 (2005); Eur. Phys. J. C **42**, 73 (2005); Proc. Sci. LAT2005 (2006) 072; Eur. Phys. J. C **47**, 453 (2006).