

Can θ/N dependence for gluodynamics be compatible with 2π periodicity in θ ?

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In a number of field theoretical models the vacuum angle θ enters physics in the combination θ/N , where N stands generically for the number of colors or flavors, in an apparent contradiction with the expected 2π periodicity in θ . We argue that a resolution of this puzzle is related to the existence of a number of different θ dependent sectors in a finite volume formulation, which cannot be seen in the naive thermodynamic limit $V \rightarrow \infty$. It is shown that, when the limit $V \rightarrow \infty$ is properly defined, physics is always 2π periodic in θ for any integer, and even rational, values of N , with vacuum doubling at certain values of θ . We demonstrate this phenomenon in both the multiflavor Schwinger model with the bosonization technique, and four-dimensional gluodynamics with the effective Lagrangian method. The proposed mechanism works for an arbitrary gauge group. [S0556-2821(98)01717-2]

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I. INTRODUCTION

Very soon after the discovery of instantons [1] in Yang-Mills (YM) theory it became clear [2] that the latter possesses a hidden parameter θ whose effects may show up due to a nontrivial topological structure of the theory. It is believed that θ is an angular parameter, i.e., physics is periodic in θ with period 2π . In particular, the values $\theta=0$ and $\theta=2\pi$ correspond to one and the same theory. This is a direct consequence of the topological classification of the gauge theories, which is based on the assumption that fields are smooth and regular, and defined on a compactifiable manifold.

The existence of this new fundamental constant has immediately posed two difficult questions related to the so-called U(1) and strong CP problems. It has been argued by 't Hooft [3] that instantons may lead to a resolution of the U(1) problem [4]. Later, Witten and Veneziano [5] found, within the large N_c approach, that physics should depend on θ through the combination θ/N_c in order for the U(1) problem to be solved. On the other hand, a nonzero value of θ implies [6,7] a violation of CP invariance in strong interactions, which is not observed experimentally. At present there is no convincing theoretical argument as to why θ is so small. Most likely, the strong CP problem cannot be solved within the strong interaction sector of the standard model, and will not be discussed here.

In the present work we address a different, but related, question. As we mentioned earlier, a resolution of the U(1) problem suggests that θ dependence comes in the combination θ/N_c . To show this, we recall the famous Witten-Veneziano relation [5]

$$f_{\eta'}^2 m_{\eta'}^2 = 12 \frac{\partial^2 E_{vac}}{\partial \theta^2}, \quad E_{vac} \sim N_c^2 f(\theta). \quad (1)$$

Here $f_{\eta'}$ is the η' residue and E_{vac} is the energy of the YM vacuum, which is proportional to N_c^2 in large N_c limit. A resolution of the U(1) problem suggests [5] that $f_{\eta'}^2 m_{\eta'}^2 \sim N_c \times 1/N_c = O(N_c^0)$. Therefore, the right hand side of Eq. (1) should also be $O(N_c^0)$. This is exactly the case provided we accept that the function f in formula (1) is actually a function of the variable θ/N_c , rather than of θ itself. This completes the standard argument showing that the θ dependence should come in the combination θ/N_c only. There exist many other arguments [based on analyses of $2D CP^{N-1}$ model, supersymmetry (SUSY) theories, etc.] which support the conclusion that the θ angle always enters physics in a combination θ/N where N is the number of ‘‘colors’’ or ‘‘flavors,’’ depending on the model considered.

The question we want to raise (and attempt to answer) can be formulated as follows. How can one reproduce the 2π periodicity in θ (which is a strict constraint following from the topological classification) for *all* physical quantities if the *same* quantities depend on θ through the specific combination θ/N_c ? The answer to this question is well known in SUSY models [8,9], where it was shown that the 2π periodicity is recovered when a discrete number of vacuum states [N for the SU(N) group, $N-2$ for the SO(N) group, etc.] is taken into account. The existence of these states in SUSY models is a consequence of spontaneous breaking of the discrete chiral symmetry $Z_{2N_c} \rightarrow Z_2$ [for the SU(N) gauge group], which shows up via a formation of the gluino condensate. In this case, the different vacua are labeled by the θ angle as well as a discrete parameter $k=0, 1, \dots, N-1$ such that the chiral condensate depends on these parameters as $\langle \bar{\lambda} \lambda \rangle \sim \exp[(i\theta + 2\pi k)/N]$. Therefore, when θ varies continuously from 0 to 2π , N_c distinct and disconnected Bloch type vacua undergo a cyclic permutation: the first state becomes the second one, and so on. All physical quantities are periodic in θ with periodicity 2π , as these vacua can be just relabeled by the substitution $k \rightarrow k-1$ after the shift $\theta \rightarrow \theta + 2\pi$, keeping physics intact. We should note that such a picture is believed to be correct for an arbitrary gauge group,

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irrespective of the existence of the center of the group.¹

In non-supersymmetric models such a scenario apparently cannot be realized because no discrete symmetry which could lead to such degenerate vacua exists in a pure gauge theory. The main goal of the present paper is to argue that the pattern of the θ dependence in usual, non-supersymmetric YM theory (gluodynamics) is to some extent reminiscent of what happens in SUSY models, although there are important differences between these two cases.

What will be shown is that a discrete number of states, whose presence is crucial for the aforementioned mechanism to work, does exist in non-supersymmetric gluodynamics when we consider the theory in a large, albeit finite, volume V . These states represent in this case local extrema of an effective potential, and have different energies. Under the shift $\theta \rightarrow \theta + 2\pi$, they transform to each other by a cyclic permutation, while some two of them cross in energy at certain values of θ .²

Thus, the periodicity in θ with period 2π is restored in this finite volume theory. However, when the thermodynamic limit $V \rightarrow \infty$ is performed for a generic value of θ , only one state of lowest energy can be seen, as all other states have higher energies and therefore drop out in the standard definition

$$E_{vac}(\theta) = - \lim_{V \rightarrow \infty} \frac{1}{V} \log Z, \quad \theta \text{ fixed.} \quad (2)$$

(This is in drastic contrast with the SUSY case where all N_c vacua have the same vanishing energy, and thus all survive the $V \rightarrow \infty$ limit.) On the other hand, due to the superselection rule different states do not communicate to each other (and are absolutely stable), and therefore the fact of existence of additional higher energy states could be safely neglected, in agreement with Eq. (2), for all physical problems except for one. Namely, retaining all these states is necessary for the analysis of periodicity in θ . The values θ and $\theta + 2\pi$ are physically equivalent for this set of states as a whole. Thus, the fact that the θ dependence comes in the combination θ/N_c in usual $V = \infty$ formulas has nothing to do with the problem of periodicity in θ , as those formulas refer to one particular state out of this set. As for any fixed θ the information on all additional states is lost in Eq. (2), in what follows this phenomenon will be referred to as a ‘‘noncommutativity’’ of the thermodynamic limit $V \rightarrow \infty$ and the shift $\theta \rightarrow \theta + 2\pi$. Bearing in mind that the states of the set do not interact owing to the superselection rule, and to have a correspondence with the standard definition (2), in what follows we call the true vacuum state a state of lowest energy (for a

fixed θ) among this set. When defined in this way, the physical vacuum is periodic in θ with period 2π , but for different intervals of the values of θ we are talking about a different state from the set as a true vacuum. At certain values of θ an exact twofold degeneracy in this set results in vacuum doubling in the limit $V \rightarrow \infty$ (Dashen phenomenon [18]).

As a warm-up example, we first discuss in Sec. II the multiflavor Schwinger model. Using the bosonization approach, we show that the θ dependence is realized in this model in the way just described. An important role of an integer valued Lagrange multiplier field, ensuring the quantization of the topological charge, is clarified.

The rest of the paper is devoted to the problem of θ dependence in four dimensional YM theory. To this end, the knowledge of an infinite series of zero momentum correlation functions of the topological density $G_{\mu\nu}\tilde{G}_{\mu\nu}$ is required. We discuss in Sec. III methods for getting information of this sort by matching short distance and large distance properties of the theory (a related discussion can be found in the Appendix). We then construct in Sec. IV an effective Lagrangian (more precisely, effective potential) as the (Legendre transform of) generating functional for zero momentum correlation functions of the marginal operators $G_{\mu\nu}\tilde{G}_{\mu\nu}$ and $G_{\mu\nu}G_{\mu\nu}$. We show that an integer valued Lagrange multiplier field should be introduced in this effective potential to ensure a single-valuedness and boundness from below. The presence of this field imposes global quantization conditions on the fields of the effective theory, which reflect the topological charge quantization in the original YM action. Section V deals with the minimization of an ‘‘improved’’ effective potential obtained by adding this Lagrangian multiplier field to the theory. We show that this procedure yields the above picture of 2π periodicity in θ , in close analogy to what we find in the multiflavor Schwinger model. Conclusions and some discussion are presented in Sec. VI.

II. θ DEPENDENCE IN N -FLAVOR SCHWINGER MODEL

The main goal of this section is to illustrate most essential technical tools, needed to address the problem of θ dependence in YM theory, on a simple toy model. The multiflavor Schwinger model nicely serves this purpose. It exhibits the above pattern of θ dependence and can be analyzed in quite a straightforward manner. Though most of the results presented in this section are not new, we hope that this discussion may help to understand the mechanism ensuring the 2π periodicity in θ in a more complicated case of four dimensional YM theory.

As is known [19,20], in the N flavor Schwinger model physics depends on θ through the combination θ/N . At the same time, all physical quantities are periodic functions of θ with period 2π . We here wish to discuss the way in which these two apparently contradictory facts become compatible. In what follows we reproduce some of the results of Refs. [19,20] using an approach which emphasizes a key role of an integer-valued Lagrange multiplier field and thermodynamic limit procedure in this problem.

We start with the standard Euclidean action of the

¹A related question on a role of the torons [10–14], which are field configurations with a fractional topological charge, is not addressed in this paper; see Ref. [13] for a list of related problems and discussions.

²This picture of the θ dependence is similar to the one advocated by Crewther [15], Witten [16], and Di Vecchia and Veneziano [17] for QCD with N_f light flavors.

bosonized one flavor Schwinger model. It takes the form

$$S_E = \int d^2x \left[\frac{1}{2g^2} F^2 + \frac{1}{2} (\partial_\mu \phi)^2 + \frac{i}{\sqrt{\pi}} F \phi - \mu m_q \cos(\sqrt{4\pi} \phi) + \frac{iF\theta}{2\pi} \right], \quad (3)$$

where $F = \frac{1}{2} \epsilon_{\mu\nu} F_{\mu\nu}$ and m_q is a quark mass. In obtaining this formula we used the standard boson-fermion correspondence

$$\bar{\psi} \gamma_\mu \psi \rightarrow \frac{1}{\sqrt{\pi}} \epsilon_{\mu\nu} \partial_\nu \phi, \quad \bar{\psi} \psi \rightarrow -\mu \cos(\sqrt{4\pi} \phi). \quad (4)$$

The key observation is the following. We would like to impose explicitly a global constraint ensuring that the topological charge, which is determined by the integral $\int d^2x (F/2\pi)$, can take only integer values. This constraint can be imposed by introducing an integer-valued Lagrange multiplier variable n such that the partition function of the theory is *defined* as the sum over n :

$$Z = \sum_n \int DFD \phi e^{-S_E + in2\pi} \int d^2x (F/2\pi). \quad (5)$$

It is clear that we have done nothing wrong by defining the partition function in this way, because we introduced only a phase multiplier which always equals 1 for integer topological charges. This procedure brings a divergent normalization factor $\sum 1$ which is irrelevant anyhow.

Two remarks are in order. First, the constraint $\int d^2x (F/2\pi) = l$, $l = 0, \pm 1, \pm 2, \dots$ is automatically satisfied due to the identity:

$$\sum_n \exp\left(i2\pi n \int d^2x \frac{F}{2\pi}\right) = \sum_l \delta\left(\int d^2x \frac{F}{2\pi} - l\right). \quad (6)$$

As for the second, and most important, remark: the 2π periodicity in θ is explicitly seen from the general expression (5). Indeed, a shift in θ by 2π in Eq. (3) can be compensated for by a shift in n : $n \rightarrow n+1$ such that the partition function (5) is unchanged. The crucial point to make this mechanism work is the definition (5) of the partition function Z with the prescription of summing over all n . Such a definition was suggested earlier (with quite a different motivation) for the Schwinger model by Smilga [21], and for SUSY models (with purposes similar to ours) by Kovner and Shifman [9].

To study the vacuum structure of the theory, we expand, following Ref. [21], the fields $F(x)$ and $\phi(x)$ in the series over spherical harmonics (a compactification on a manifold of volume V is implied) $F(x) = \sum F_{lm} Y_{lm}(\Omega)$, $\phi(x) = \sum \phi_{lm} Y_{lm}(\Omega)$ and keep only the zero F_0 mode in what follows. This harmonic $F_0 = 2\pi l/V$ is fixed by the constraint (6), with V being the total volume of the system. Integrating over DF_0 and discarding non-zero harmonics of the ϕ field, which are irrelevant for the present discussion, we obtain for the partition function

$$Z \sim \int_{-\sqrt{\pi}/2}^{+\sqrt{\pi}/2} D\phi_0 \sum_{l=-\infty}^{+\infty} \exp\left\{ -\frac{2\pi^2 l^2}{Vg^2} + il(\sqrt{4\pi}\phi_0 + \theta) + Vm_q \mu \cos(\sqrt{4\pi}\phi_0) \right\}. \quad (7)$$

The 2π periodicity in θ is explicitly seen in this representation. However, in order to discuss the thermodynamic limit, it is more convenient to use an alternative (dual) representation for the same expression (7):

$$Z \sim \int_{-\sqrt{\pi}/2}^{+\sqrt{\pi}/2} D\phi_0 \sum_{k=-\infty}^{+\infty} \exp\left\{ -\frac{g^2 V}{2\pi} \left(\phi_0 - k\sqrt{\pi} + \frac{\theta}{\sqrt{4\pi}} \right)^2 + Vm_q \mu \cos(\sqrt{4\pi}\phi_0) \right\}, \quad (8)$$

where we have used the property of $\theta_3(\nu, x)$ function:

$$\theta_3(\nu, x) = \frac{1}{\sqrt{\pi x}} \sum_{k=-\infty}^{+\infty} e^{-(\nu+k)^2/x} = \sum_{l=-\infty}^{+\infty} e^{-l^2 \pi^2 x + 2il\nu\pi}. \quad (9)$$

A generalization of this formula for the case of N_f flavors with equal (and very small, $m_q \ll g$) masses can be achieved by replacing $\phi_0 \rightarrow N_f \phi_0$ in Eq. (8) where, again, we keep only the relevant for the vacuum structure part of the partition function:

$$Z \sim \int_{-\sqrt{\pi}/2}^{+\sqrt{\pi}/2} D\phi_0 \sum_{k=-\infty}^{+\infty} \exp\left\{ -\frac{g^2 V}{2\pi} \left(N_f \phi_0 - k\sqrt{\pi} + \frac{\theta}{\sqrt{4\pi}} \right)^2 + Vm_q \mu N_f \cos(\sqrt{4\pi}\phi_0) \right\}. \quad (10)$$

Formula (10) was derived earlier [21] in the limit $\theta=0, N_f=1$.

Now we are ready to discuss the periodic properties of the partition function (10) in the thermodynamic limit $g^2 V \rightarrow \infty$ for the strong coupling regime $m_q \ll g$. It is clear beforehand, without any calculations, that Z is a periodic function of θ with period 2π for an arbitrary N_f , due to summation over the integers k in Eq. (10). Now we wish to see explicitly how this periodicity works in Eq. (10) in the limit $g^2 V \rightarrow \infty$. For sufficiently small θ , only one term $k=0$ in the sum (10) survives the thermodynamic limit, such that

$$\sqrt{4\pi}\phi_0 = -\frac{\theta}{N_f}, \quad g^2 V \rightarrow \infty, \quad k=0, \quad 0 \leq \theta < \pi. \quad (11)$$

The vacuum energy and topological density condensate for solution (11) are

$$E_{vac}(\theta) \sim -\cos(\sqrt{4\pi}\phi_0) \sim -\cos\frac{\theta}{N_f}$$

$$\left\langle \frac{iF}{2\pi} \right\rangle \sim \sin\frac{\theta}{N_f}, \quad 0 \leq \theta < \pi. \quad (12)$$

When $\theta > \pi$, the next term with $k=1$ corresponds to a lowest energy state, such that

$$\sqrt{4\pi}\phi_0 = \frac{2\pi}{N_f} - \frac{\theta}{N_f}, \quad g^2 V \rightarrow \infty, \quad k=1, \quad \pi < \theta \leq 2\pi. \quad (13)$$

The vacuum energy and topological density condensate for solution (13) are

$$E_{vac}(\theta) \sim -\cos(\sqrt{4\pi}\phi_0) \sim -\cos\left(\frac{2\pi}{N_f} - \frac{\theta}{N_f}\right)$$

$$\left\langle \frac{iF}{2\pi} \right\rangle \sim -\sin\left(\frac{2\pi}{N_f} - \frac{\theta}{N_f}\right), \quad \pi < \theta \leq 2\pi. \quad (14)$$

This pattern continues for arbitrary values of θ . For the special case $\theta = \pi$, a cusp singularity develops, and we stay with two degenerate vacua which both survive the thermodynamic limit (the phenomenon of vacuum doubling in the massive Schwinger model was first found long ago by Coleman [19] for the case $N_f=1$, $m_q \gg g$). In this case the two vacua are distinguished by the sign of the topological density condensate $\langle iF/(2\pi) \rangle$.

To summarize, we explicitly see that physics depends on θ for sufficiently small θ through the combination θ/N_f . At the same time, the period of the θ dependence is standard 2π . This result is in agreement with a very different approach of Ref. [20].

We thus see that the following picture emerges.

(1) The 2π periodicity in θ holds for an arbitrary value of N_f , even if N_f is a rational, and not an integer, number (thought it is not a physical situation for the Schwinger model, a similar formula for four-dimensional gluodynamics exhibits such a possibility). The 2π periodicity in θ is always restored due to the summation over integer-valued Lagrange multiplier variable n in the partition function (5).

(2) If we take the thermodynamic limit for sufficiently small θ in Eq. (10) from the very beginning, we obtain $\sqrt{4\pi}\phi_0 = -\theta/N_f$ once and forever for an arbitrary value of θ . Proceeding this way, we would not see other terms with $k=1, 2 \dots$ in Eq. (10), which are responsible for the restoration of 2π periodicity in θ , simply because they contribute zero to the partition function in the thermodynamic limit. This is exactly what happens when one starts with the continuum formulation of the theory from the very beginning. In this case all terms with $k=1, 2 \dots$ are automatically discarded. Therefore, the 2π periodicity in θ , as a property of the whole set of solutions, cannot be seen in this formulation. The thermodynamic limit prescription (2) and the shift $\theta \rightarrow \theta + 2\pi$ are thus ‘‘noncommutative.’’

(3) For each given $\theta \neq \pi$ (and $m_q \neq 0$) there is one and only one physical vacuum in the thermodynamic limit. By

convention (2) we define this vacuum as a state of lowest energy among the above set. For $\theta = \pi$ there are exactly two degenerate states which both contribute the partition function in the limit $V \rightarrow \infty$. In this sense, at the crossing point $\theta = \pi$ the physics is nonanalytic in θ . This nonanalyticity cannot be seen in usual $V = \infty$ formulas valid for small $\theta < \pi$, where a contribution of a lowest energy state only is retained. An order parameter which labels two degenerate states at $\theta = \pi$ is the sign of the vacuum expectation value of operator $\langle iF/2\pi \rangle \sim \pm m_q \sin(\pi/N_f)$.

(4) As we mentioned above, the choice of the physical vacuum as a lowest energy state is a matter of convention. Owing to the superselection rule, any state in the discrete series (e.g., a next-to-lowest state) could serve as a vacuum as well. However, due to the permutational symmetry of the whole set of states under the shift $\theta \rightarrow \theta + 2\pi$, any redefinition of this sort will result in 2π periodicity in θ for such a vacuum in the physical limit $V \rightarrow \infty$.

In the next sections we will see that the very same picture of the physical θ dependence seems to appear in four dimensional YM theory.

III. LOW ENERGY THEOREMS IN GLUODYNAMICS

In this section we start to describe steps which have to be done in YM theory to obtain an expression analogous to Eq. (10) for the Schwinger model (the vacuum contribution to the partition function or, in other words, the vacuum energy). This aim requires knowing the zero momentum part of the YM partition function, which cannot be described within perturbation theory. It turns out that this object can be studied using some matching conditions ensuring consistency of the large distance properties of the theory with its small distance behavior fixed by renormalizability and asymptotic freedom. These matching conditions are provided by anomalously broken symmetries through a set of Ward identities³ for zero momentum correlation functions of operators describing corresponding anomalies. This constitutes what is known as low energy theorems in gluodynamics. Our aim in this section is to discuss the low energy theorems in YM theory in order to prepare a necessary input for the construction of an effective Lagrangian, which will be carried out in Sec. IV.

In what follows we need two Ward identities for zero momentum correlation functions of spin 0 gluon currents in gluodynamics. For the scalar channel case, it was shown long ago by Novikov *et al.* [23] (NSVZ) that these correlation functions are fixed by renormalizability and conformal anomaly in YM theory. Indeed renormalizability and dimensional transmutation ensure that any renormalized zero momentum correlation function of the $d=D=4$ operator G^2 can only be of the form $C \langle \beta(\alpha_s)/(4\alpha_s)G^2 \rangle$, where C is a numerical constant which depends on the correlation function considered, and the renormalized vacuum expectation

³In SUSY models, a similar use of anomalous Ward identities leads to the well known Veneziano-Yankielowicz effective Lagrangian [22].

value $\langle \beta(\alpha_s)/(4\alpha_s G^2) \rangle \sim \Lambda_{YM}^4$ is the only mass scale in the theory, fixed by the conformal anomaly.⁴ For any given zero momentum correlation function of the field G^2 , a value of the particular coefficient C can be found using the dimensional transmutation formula for renormalized vacuum expectation value of operator O of canonical dimension d , written in terms of the bare coupling constant g_0 normalized at the cut-off scale M_R :

$$\langle O \rangle = \text{const} \left[M_R \exp \left(- \frac{8\pi^2}{bg_0^2} \right) \right]^d, \quad (15)$$

where the one-loop β -function, $\beta(\alpha_s) = -b\alpha_s^2/(2\pi)$ with $b = (11/3)N_c$ and N_c stands for the number of colors, has been used. The NSVZ theorem [23] (with the one-loop β function) then follows by the differentiation of Eq. (15), taken for $O = -b\alpha_s/(8\pi)G^2$, in respect to $1/g_0^2$. When the full β function is retained, it reads [23]

$$\begin{aligned} \lim_{q \rightarrow 0} i \int dx e^{iqx} \langle 0 | T \left\{ \frac{\beta(\alpha_s)}{4\alpha_s} G^2(x) \frac{\beta(\alpha_s)}{4\alpha_s} G^2(0) \right\} | 0 \rangle \\ = -4 \left\langle \frac{\beta(\alpha_s)}{4\alpha_s} G^2 \right\rangle. \end{aligned} \quad (16)$$

Note that the presence of the full β function in Eq. (16) ensures the renormalization group invariance of both sides of this relation. An infinitesimally small momentum transfer q_μ is introduced in order to select a connected contribution to the correlation function (16). Equation (16) stands for the renormalized correlation function where ultraviolet divergent contributions are implied to be regularized and subtracted in both sides of Eq. (16), see the Appendix for a discussion on this point.

Arbitrary n -point functions of the trace of the energy-momentum tensor

$$\langle \sigma \rangle = \left\langle \frac{\beta(\alpha_s)}{4\alpha_s} G^2 \right\rangle = \left\langle \frac{-b\alpha_s}{8\pi} G^2 \right\rangle + O(\alpha_s^2) \quad (17)$$

can be obtained by further differentiating relation (15):

$$\begin{aligned} i^n \int dx_1 \dots dx_n \langle 0 | T \{ \sigma(x_1) \dots \sigma(x_n) \sigma(0) \} | 0 \rangle \\ = (-4)^n \langle \sigma \rangle, \end{aligned} \quad (18)$$

where, as in Eq. (16), a limiting procedure of the vanishing momentum transfer q_μ is implied. Note that a regularization scheme in Eqs. (16),(18) is assumed to be the same.

Let us now address zero momentum correlation functions of the topological density operator in gluodynamics. As discussed in detail in the Appendix, the renormalized two-point function can be written as

$$\begin{aligned} \lim_{q \rightarrow 0} i \int dx e^{iqx} \langle 0 | T \left\{ \frac{\alpha_s}{8\pi} G\tilde{G}(x) \frac{\alpha_s}{8\pi} G\tilde{G}(0) \right\} | 0 \rangle \\ = \xi^2 \left\langle \frac{\beta(\alpha_s)}{4\alpha_s} G^2 \right\rangle, \end{aligned} \quad (19)$$

where ξ stands for a generally unknown numerical coefficient [note that its N_c dependence is expected to be $\xi \sim N_c^{-1}$, in order to match Witten-Veneziano [5] resolution of the U(1) problem]. When $\theta=0$, Eq. (19) is the only possible form compatible with both the conformal anomaly and Witten-Veneziano construction. We note that the correlation function (19) is defined via the path integral, i.e., with Wick type of the T-product. This definition ensures that the non-perturbative gluon condensate in Eqs. (16),(19) is the same quantity. Perturbative contributions are absent in Eq. (19), see the Appendix.

In writing Eq. (19) we have assumed that it has the same form, i.e., covariant, for any small value of θ (in the Appendix it is proved only for $\theta=0$). Provided this is the case, the coefficient ξ^2 reiterates, analogously to Eq. (18), for all n -point correlation functions of $G\tilde{G}$, as can be seen by the formal differentiation of Eq. (19) in respect to θ . There are three arguments in favor of correctness of this assumption. First, this requirement agrees with the large N_c line of reasoning due to Veneziano [5] where one finds that a coefficient standing in the two-point function of the topological density operator does reiterate in multipoint correlation functions. Second, this postulated covariance of Eq. (19) in respect to θ goes through a self-consistency check by agreement between two different calculations of the θ dependence of the vacuum energy, when one of them is obtained by a straightforward use of Eq. (19) [see Eq. (20) below], and another one is obtained directly from an effective potential (see Sec. V). Third, such covariance of Eq. (19) follows automatically with an approach used in [24].

As for the numerical coefficient ξ in Eq. (19), there exist a few proposals to fix its value. One of them [23] is based on the hypothesis of the dominance of self-dual fields in the YM vacuum, which suggests $\xi = 2/b$. A different choice, $\xi = 4/(3b)$, was advocated in our work [24] using a one-loop connection between the conformal and axial anomalies in the theory with an auxiliary heavy fermion. This line of reasoning was an extension of arguments used by Kühn and Zakharov [25] to evaluate the proton matrix element $\langle p | G\tilde{G} | p \rangle$. Some further discussion on these matters will be given in Sec. V. As different arguments disagree on what the exact value of ξ is, in this paper we prefer to proceed with an unspecified parameter ξ . Fortunately, it turns out that the fact of 2π periodicity in θ can be established without knowing a precise value of ξ , with the only mild and reasonable assumption that the parameter ξ is a rational number. In addition, keeping an unspecified value of ξ in Eq. (19) makes it possible to study the θ dependence for gauge groups other than SU(N), at least in principle (see Sec. V).

As has been shown in [24], a combined use of relations (16),(19) enables us to calculate the θ dependence of the vacuum energy and topological density condensate for any

⁴The fact that terms explicitly containing Λ_{YM}^4 do not appear in correlation functions of the operator G^2 was checked in Ref. [23] using canonical methods with Pauli-Villars regularization.

number of colors N_c and small values of the vacuum angle θ by formal resummations of Taylor expansions in θ for these objects. The resulting expressions read

$$\begin{aligned} E_v(\theta) &= \langle \theta | -\frac{b\alpha_s}{32\pi} G^2 | \theta \rangle = \langle 0 | -\frac{b\alpha_s}{32\pi} G^2 | 0 \rangle \cos(2\xi\theta) \\ &\equiv E_v \cos(2\xi\theta) \end{aligned} \quad (20)$$

for the vacuum energy (here E_v stands for the vacuum energy for $\theta=0$) and

$$\langle \theta | \frac{\alpha_s}{8\pi} G\tilde{G} | \theta \rangle = 2\xi E_v \sin(2\xi\theta) \quad (21)$$

for the topological density condensate [in [24] the particular value $\xi=4/(3b)$ was used]. These formulas seem puzzling as they suggest a ‘‘wrong’’ periodicity in θ (remember that $\xi \sim N_c^{-1}$) without any hint at possible singular points $\theta \sim \pi$, which could prevent us from making the shift $\theta \rightarrow \theta + 2\pi$. This might force one to conclude that Eqs. (20),(21) cannot be correct on general grounds, even for small values of θ , and the whole derivation, leading to relations (20),(21), was in error. However, as we just saw in the analysis of the Schwinger model, a fractional θ dependence, implied in Eqs. (20),(21), can be in perfect agreement with the 2π periodicity in θ , see Eq. (12). What will be argued below is that Eqs. (20),(21) do *not* contradict the expected picture of 2π periodicity of physics in θ with a singular level crossing point at $\theta \sim \pi$, for any rational number ξ [including, of course, both aforementioned choices $\xi=2/b$ [23] or $\xi=4/(3b)$ [24]]. As we have found in the study of the Schwinger model, the key to understanding the θ periodicity problem is the analysis of a whole set of disconnected vacuum states. It will be shown in Sec. V that an accurate transition to the limit $V \rightarrow \infty$ while keeping all these states restores the correct periodicity and analyticity structure of the θ dependence, irrespective of a particular value $\xi = \text{any rational number}$.

IV. EFFECTIVE LAGRANGIAN FOR GLUODYNAMICS

The purpose of this section is to construct a low energy effective Lagrangian for gluodynamics, which would contain all information provided by the low energy theorems in the scalar (16) and pseudoscalar (19) channels including all multi-point correlation functions of operators G^2 and $G\tilde{G}$, which can be obtained by differentiating the two-point functions (16) and (19), see e.g. Eq. (18).

Before proceeding with the presentation, we would like to pause for a comment on the meaning of this effective Lagrangian. As there exist no Goldstone bosons in pure YM theory, no Wilsonian effective Lagrangian, which would correspond to integrating out heavy modes, can be constructed for gluodynamics. Instead, one speaks in this case of an effective Lagrangian as a generating functional for vertex functions of the composite fields G^2 and $G\tilde{G}$. Moreover, only the potential part of this Lagrangian can be found as it corresponds to zero momentum n-point functions of $G^2, G\tilde{G}$, fixed by the low energy theorems. (This effective potential

still contains an ambiguity which will play an important role in what follows.) The kinetic part is not fixed in this way. Thus, such an effective Lagrangian is not very useful for calculating the S-matrix, but is perfectly suitable for addressing the vacuum properties.⁵ Specifically, space-time independent fields are amenable to a study within this framework.

The task of constructing an effective Lagrangian can be considerably simplified by going over to linear combinations of original operators⁶ which enter relations (16), (19):

$$\begin{aligned} H &= \frac{b}{64\pi^2} \left(-G^2 + i \frac{2}{b\xi} G\tilde{G} \right), \\ \bar{H} &= \frac{b}{64\pi^2} \left(-G^2 - i \frac{2}{b\xi} G\tilde{G} \right). \end{aligned} \quad (22)$$

In terms of these combinations, the low energy theorems for renormalized zero momentum Green function, Eqs. (16) and (19), take particularly simple forms (for an arbitrary value of the vacuum angle θ):

$$\begin{aligned} \lim_{q \rightarrow 0} i \int dx e^{iqx} \langle 0 | T \{ H(x) H(0) \} | 0 \rangle &= -4 \langle H \rangle, \\ \lim_{q \rightarrow 0} i \int dx e^{iqx} \langle 0 | T \{ \bar{H}(x) \bar{H}(0) \} | 0 \rangle &= -4 \langle \bar{H} \rangle, \quad (23) \\ \lim_{q \rightarrow 0} i \int dx e^{iqx} \langle 0 | T \{ \bar{H}(x) H(0) \} | 0 \rangle &= 0. \end{aligned}$$

It is easy to check that the decoupling of the fields H and \bar{H} holds for arbitrary n-point functions of H, \bar{H} . This circumstance makes it particularly convenient to work with fields (22).

We now wish to construct an effective low energy Lagrangian reproducing at the tree level all Ward identities (low energy theorems) for the composite fields H, \bar{H} , such as Eqs. (23) and their n-point generalizations.⁷ To this end, we consider the generating functional of connected Green functions with the space-time independent sources J, \bar{J}

⁵Effective Lagrangians of this kind have been used in supersymmetric theories (see, e.g., review papers [26]). In particular, the so-called Veneziano-Yankielowicz effective Lagrangian [22] has the meaning just described; see [9].

⁶In this section we change the normalization of the gluon field in comparison to that used in Sec. III by the rescaling $A_\mu \rightarrow (1/g)A_\mu$, and use the one-loop β function.

⁷For the case of one real ‘‘dilaton’’ fields $\sigma = -b\alpha_s/(8\pi)G^2$, a similar problem of constructing an effective Lagrangian was solved long ago by Schechter [27], and Migdal and Shifman [28] (see also [29]). Our derivation below is akin to the one suggested by Cornwall and Soni in [29].

$$\begin{aligned} \exp[iW(J,\bar{J})] = \sum_n \int DA \exp \left[-\frac{i}{4g^2} \int dx G^2 \right. \\ \left. + i \frac{\theta + 2\pi n}{32\pi^2} \int dx G\tilde{G} + iJ \int dx H \right. \\ \left. + i\bar{J} \int dx \bar{H} \right]. \end{aligned} \quad (24)$$

Note the (somewhat unconventional) summation over all integer numbers n in Eq. (24), which is analogous to the definition (5) for the Schwinger model. This prescription automatically ensures the 2π periodicity in θ and quantization of the topological charge, and is completely equivalent to the way the vacuum angle θ has initially appeared in YM theory [2]. The above form of introducing the θ angle in the path integral will help us to understand how the θ parameter should be installed in the effective Lagrangian formalism.

We next define the effective zero momentum fields (here and in what follows $\int dx = V$ is a total 4-volume)

$$\int dx h = \frac{\partial W}{\partial J}, \quad \int dx \bar{h} = \frac{\partial W}{\partial \bar{J}}, \quad (25)$$

satisfying the equations

$$\int dx h = \left\langle \int dx H \right\rangle, \quad \int dx \bar{h} = \left\langle \int dx \bar{H} \right\rangle. \quad (26)$$

The effective action $\Gamma(h,\bar{h})$ is now introduced as the Legendre transform of the generating functional $W(J,\bar{J})$:

$$\Gamma(h,\bar{h}) = -W(J,\bar{J}) + \int dx Jh + \int dx \bar{J}\bar{h} \quad (27)$$

which implies

$$\frac{\partial \Gamma}{\partial \int dx h} = J, \quad \frac{\partial \Gamma}{\partial \int dx \bar{h}} = \bar{J}. \quad (28)$$

From the definition (24) and the low energy theorems (23) [and their extensions for arbitrary n-point functions; see Eq. (18)] we obtain

$$\begin{aligned} \frac{\partial^{n+1}}{\partial J^{n+1}} W|_{J=\bar{J}=0} = i^n \int dx dx_1 \dots dx_n \\ \times \langle T\{H(x_1) \dots H(x_n)H(0)\} \rangle \\ = (-4)^n \int dx \langle H \rangle \end{aligned}$$

$$\begin{aligned} \frac{\partial^{n+1}}{\partial \bar{J}^{n+1}} W|_{J=\bar{J}=0} = i^n \int dx dx_1 \dots dx_n \\ \times \langle T\{\bar{H}(x_1) \dots \bar{H}(x_n)\bar{H}(0)\} \rangle \\ = (-4)^n \int dx \langle \bar{H} \rangle \end{aligned}$$

$$\frac{\partial^{k+l}}{\partial J^k \partial \bar{J}^l} W|_{J=\bar{J}=0} = 0; \quad (29)$$

[as before, the connected parts of the Green functions are implied in Eq. (29)]. These equations are solved by the function

$$W(J,\bar{J}) = -\frac{1}{4} \int dx \langle H \rangle e^{-4J} - \frac{1}{4} \int dx \langle \bar{H} \rangle e^{-4\bar{J}}. \quad (30)$$

Using Eq. (25), we can express the sources J,\bar{J} in terms of the fields h,\bar{h} :

$$J = -\frac{1}{4} \log \left(\frac{h}{\langle H \rangle} \right), \quad \bar{J} = -\frac{1}{4} \log \left(\frac{\bar{h}}{\langle \bar{H} \rangle} \right). \quad (31)$$

Inserting these expressions back to Eq. (30), we obtain W as a function of the fields h,\bar{h} . Now the definition (27) turns into the differential equation for the effective potential $U(h,\bar{h}) = -(1/V)\Gamma(h,\bar{h})$:

$$U - h \frac{\partial U}{\partial h} - \bar{h} \frac{\partial U}{\partial \bar{h}} = -\frac{1}{4}(h + \bar{h}). \quad (32)$$

This equation is a complex extension of a real differential equation for the ‘‘dilaton’’ effective potential of Refs. [27,28]. Here comes the aforementioned ambiguity of the effective potential. Let us compare Eq. (32) with the equation for the real ‘‘dilaton’’ field of [27,28]

$$U(\sigma) - \sigma \frac{dU}{d\sigma} = -\frac{1}{4}\sigma. \quad (33)$$

Equation (33) has the only solution $U(\sigma) = (1/4)\sigma(\log \sigma + \text{const})$. It is the appearance of the multibranched logarithmic function of a complex argument in Eq. (32) that gives rise to the ambiguity which was absent in the real equation (33). Let us analyze the way it appears when Eq. (32) is solved. One obvious solution of Eq. (32) is

$$U_1(h,\bar{h}) = \frac{1}{4} h \log \frac{h}{C} + \frac{1}{4} \bar{h} \log \frac{\bar{h}}{\bar{C}} + D(h - \bar{h}), \quad (34)$$

where C,\bar{C},D are arbitrary complex constants which may depend on $\langle H \rangle, \langle \bar{H} \rangle, \theta$. However, Eq. (34) is not a single-valued function, and is not bounded from below. After the phase rotation $h \rightarrow h \exp(2\pi i r)$ with an arbitrary integer r , the potential (34) transforms as

$$U_1(h, \bar{h}) \rightarrow U_1(h, \bar{h}) + \frac{i\pi r}{2}(h - \bar{h}) \quad (35)$$

which is physically unacceptable.

A way out in this situation is to sum over all integers r in the partition function, as was suggested by Kovner and Shifman [9] in a similar problem arising with Veneziano-Yankielowicz effective Lagrangian [22] for SUSY gluodynamics. Yet, in our case this is not the end of the story. Indeed we find that there exists another possible solution of Eq. (32):

$$U_2(h, \bar{h}) = \frac{1}{4\alpha} h \log\left(\frac{h}{C}\right)^\alpha + \frac{1}{4\alpha} \bar{h} \log\left(\frac{\bar{h}}{\bar{C}}\right)^\alpha + D(h - \bar{h}), \quad (36)$$

where α is an arbitrary real number. From now on we concentrate on the case when α is a positive rational number, $\alpha = p/q$, where the integers p and q are relatively prime. Using the formula

$$\log z^{p/q} = \frac{p}{q} \text{Log } z + 2\pi i \left(n + k \frac{p}{q} \right), \quad (37)$$

$$n = 0, \pm 1, \dots; \quad k = 0, 1, \dots, q-1$$

(here \log stands for the principal branch of the logarithm), we see that the second form (36) makes no difference in comparison with Eq. (34) when only the principal value of the logarithm is considered. However, the theories, described by the effective potentials (34) and (36), are different quantum mechanically as they imply different rules of a global quantization for the fields h, \bar{h} . This quantization arises when the single-valuedness of the partition function is ensured by a summations over the integers. As will be shown in the next section, it is the second choice (36) for the effective potential that can be made consistent with both the θ/N dependence and 2π periodicity in θ when a proper treatment to global quantization constraints and the thermodynamic limit is given.

We therefore consider the function

$$U_3(h, \bar{h}) = \frac{1}{4} h \text{Log} \frac{h}{C} + \frac{1}{4} \bar{h} \text{Log} \frac{\bar{h}}{\bar{C}} + \frac{i\pi}{2} \left(k + n \frac{q}{p} \right) (h - \bar{h}), \quad (38)$$

which satisfies Eq. (32) [i.e., the Ward identities (23) and their n -point generalizations] for any values of the integers n, k from the range $n = 0, \pm 1, \dots; k = 0, 1, \dots, q-1$. The last term in Eq. (38) is a particular form of the last term $\sim D$ in Eq. (36). It can be seen that arbitrary values of the coefficient D would be incompatible with the quantization rules imposed by the summation over the integers n, k in the partition function.

Finally, we have to figure out how the θ angle should be installed in the effective potential (38). An answer to this question can be deduced by comparing with Eq. (24). In the YM partition function, the θ angle enters in the combination

$\theta + 2\pi n$, while the summation over the integers n is necessary because of a multivaluedness of the YM action in respect to large gauge transformations. Analogously, the last term in Eq. (38) is the only one that can accommodate the θ parameter in the same combination $\theta + 2\pi n$. The summation over the integers n is enforced this time by the multivaluedness of the logarithm in Eq. (38). As the presence of the θ angle is implicit in the constants C, \bar{C} , we now make it explicit in the above way and finally obtain the (Minkowsky space) improved effective potential $F(h, \bar{h})$ by the summation over n, k in the partition function:

$$e^{-iVF(h, \bar{h})} = \sum_{n=-\infty}^{+\infty} \sum_{k=0}^{q-1} \exp\left\{ -\frac{iV}{4} \left(h \text{Log} \frac{h}{C'} + \bar{h} \text{Log} \frac{\bar{h}}{\bar{C}'} \right) + i\pi V \left(k + \frac{q}{p} \frac{\theta + 2\pi n}{2\pi} \right) \frac{h - \bar{h}}{2i} \right\}, \quad (39)$$

where the constants C', \bar{C}' are independent of θ and can be taken real, $C' = \bar{C}' \equiv 2eE$, where E is some positive constant. The improved effective potential $F(h, \bar{h})$ is consistent with all constraints imposed by the low energy theorems and, by construction, is a single valued function possessing the 2π periodicity in θ , which was present in the initial YM partition function. As is seen from Eq. (39), the structure of the effective potential F is such that it contains both the ‘‘dynamical’’ and ‘‘topological’’ parts (the first and the second terms in the exponent, respectively). We would like to note that Eq. (39) is a direct analog of a similar construction for SUSY models [22,9]. Namely, the ‘‘dynamical’’ part of the effective potential is rather similar to Veneziano-Yankielowicz (VY) [22] potential $\sim u^{2/3} \log u$, while the ‘‘topological’’ part is analogous to an improvement of the VY effective potential, suggested by Kovner and Shifman [9]. We stress that the improved effective potential (39) contains more information in comparison to that present in the Ward identities (23) just due to the appearance of this ‘‘topological’’ part in Eq. (39). Without this term Eq. (39) would merely be a kinematical reformulation of the content of the Ward identities (23). As will be shown in the next section, this improvement of the effective potential turns out crucial for unravelling the correct periodicity in θ in YM theory.

V. MINIMIZATION OF EFFECTIVE POTENTIAL

In this section a ground state of the dual low energy theory will be determined by a minimization of the improved effective potential (IEP) $F(h, \bar{h})$ given by Eq. (39). Our purpose is to find the θ dependence of the vacuum energy which is defined as a minimum of IEP $F(h, \bar{h})$. In this calculation the total space-time 4-volume will be kept finite, while a transition to the thermodynamic limit $V \rightarrow \infty$ will be performed at the very end.

We start with introducing the ‘‘physical’’ real fields ρ, η defined by the relations

$$h = 2Ee^{\rho+i\eta}, \quad \bar{h} = 2Ee^{\rho-i\eta}. \quad (40)$$

[This definition implies $F(\eta + 2\pi) = F(\eta)$. As will be seen, this condition of single-valuedness of the η field is satisfied with the substitution (40).] In these variables, the ‘‘dynamical’’ part of Eq. (39) can be written as follows:

$$\begin{aligned} & -\frac{iV}{4} \left(h \operatorname{Log} \frac{h}{2eE} + \bar{h} \operatorname{Log} \frac{\bar{h}}{2eE} \right) \\ & = -iVEe^\rho [(\rho - 1) \cos \eta - \eta \sin \eta]. \end{aligned} \quad (41)$$

The summation over the integers n in Eq. (39) enforces the quantization rule due to the Poisson formula

$$\sum_n \exp \left(2\pi i n \frac{q}{p} V \frac{h - \bar{h}}{4i} \right) = \sum_m \delta \left(\frac{q}{p} VE e^\rho \sin \eta - m \right), \quad (42)$$

which reflects the quantization of the topological charge in the original theory. Therefore, when the constraint (42) is imposed, Eq. (41) can be written as

$$\begin{aligned} & -\frac{iV}{4} \left(h \operatorname{Log} \frac{h}{2eE} + \bar{h} \operatorname{Log} \frac{\bar{h}}{2eE} \right) \\ & = -iVEe^\rho (\rho - 1) \cos \eta + im \frac{p}{q} \eta. \end{aligned} \quad (43)$$

Using Eqs. (42),(43), we put Eq. (39) in the form

$$\begin{aligned} e^{-iVF} &= \sum_{m=-\infty}^{+\infty} \sum_{k=0}^{q-1} \delta \left(VE \frac{q}{p} e^\rho \sin \eta - m \right) \\ & \times \exp \left[-iVEe^\rho (\rho - 1) \cos \eta + im \left(\theta_k + \frac{p}{q} \eta \right) \right], \end{aligned} \quad (44)$$

where we denoted

$$\theta_k \equiv \theta + 2\pi \frac{p}{q} k. \quad (45)$$

To resolve the constraint imposed by the presence of the δ function in Eqs. (42),(44), we introduce the new field M by the formula

$$\begin{aligned} & \delta \left(VE \frac{q}{p} e^\rho \sin \eta - m \right) \\ & \propto \int DM \exp \left(iMVEe^\rho \sin \eta - iM \frac{p}{q} m \right). \end{aligned} \quad (46)$$

Going over to Euclidean space⁸ by the substitution $iV \rightarrow V$, we obtain from Eqs. (44),(46)

⁸This is not really necessary. All formulas below can be worked out in Minkowsky space as well.

$$\begin{aligned} F(\rho, \eta, M) &= -\frac{1}{V} \log \left\{ \sum_{m=-\infty}^{+\infty} \sum_{k=0}^{q-1} \exp \left[-VEe^\rho \right. \right. \\ & \quad \times \{ (\rho - 1) \cos \eta - M \sin \eta \} \\ & \quad \left. \left. + im \left(\theta + 2\pi k \frac{p}{q} + \frac{p}{q} \eta - \frac{p}{q} M \right) - \varepsilon \frac{m^2}{VE} \right] \right\}. \end{aligned} \quad (47)$$

Here we introduced the last term to regularize the infinite sum over the integers m . The limit $\varepsilon \rightarrow 0$ will be carried out at the end, but before taking the thermodynamic limit $V \rightarrow \infty$. Note that Eq. (47) satisfies the condition $F(\eta + 2\pi) = F(\eta)$ which should hold as long as η is an angle variable. We also note that the periodicity in θ with period 2π is explicit in Eq. (47).

Proceeding as was done for the Schwinger model, to discuss the thermodynamic limit $V \rightarrow \infty$ we use the identity (9) and transform Eq. (47) into its dual form

$$\begin{aligned} F(\rho, \eta, M) &= -\frac{1}{V} \log \left\{ \sum_{n=-\infty}^{+\infty} \sum_{k=0}^{q-1} \exp \left[-VEe^\rho \right. \right. \\ & \quad \times \{ (\rho - 1) \cos \eta - M \sin \eta \} \\ & \quad \left. \left. - \frac{VE}{4\varepsilon} \left(\theta + 2\pi k \frac{p}{q} + \frac{p}{q} \eta - \frac{p}{q} M - 2\pi n \right)^2 \right] \right\}, \end{aligned} \quad (48)$$

where we have omitted an irrelevant infinite factor $\sim \varepsilon^{-1/2}$ in front of the sum. Equation (48) is the final form of the improved effective potential F , which represents the YM analog of Eq. (10) for the Schwinger model. To discuss the vacuum properties, the function F should be minimized in respect to the three variables ρ, η and M . In spite of the frightening form of this function, its extrema can be readily found using the following simple trick. As at the extremum points all partial derivatives of the function F vanish, we first consider their linear combination in which the sum over n, k cancels out. We thus arrive at the equations

$$\frac{\partial F}{\partial \rho} = Ee^\rho (\rho \cos \eta - M \sin \eta) = 0,$$

$$\frac{\partial F}{\partial \eta} + \frac{\partial F}{\partial M} = -Ee^\rho (\rho \sin \eta + M \cos \eta) = 0, \quad (49)$$

which is equivalent to $\rho^2 + M^2 = 0$. Therefore, these equations have the only solution

$$\langle \rho \rangle = 0, \quad \langle M \rangle = 0, \quad (50)$$

while the minimum value of the angular field η is left arbitrary by them. The latter can now be found from either of the

constraints $\partial F/\partial \eta=0$ or $\partial F/\partial M=0$, which become identical for $\langle \rho \rangle = \langle M \rangle = 0$. The resulting equation reads⁹

$$\sum_{n=-\infty}^{+\infty} \sum_{k=0}^{q-1} \left(\theta + 2\pi k \frac{p}{q} - 2\pi n + \frac{p}{q} \eta + 2\varepsilon \frac{q}{p} \sin \eta \right) \times \exp \left\{ VE \cos \eta - \frac{VE}{4\varepsilon} \left(\theta + 2\pi k \frac{p}{q} + \frac{p}{q} \eta - 2\pi n \right)^2 \right\} = 0, \quad (51)$$

in which we have to take the limit $\varepsilon \rightarrow 0$ at a fixed 4-volume V .

One can see that nontrivial solutions of Eq. (51) at $\varepsilon \rightarrow 0$ are given by

$$\langle \eta \rangle_l = -\frac{q}{p} \theta + \frac{2\pi}{p} l + 2\pi r, \quad l=0,1,\dots,p-1; \quad r=0,\pm 1,\dots \quad (52)$$

Equation (52) shows that there are p physically distinct solutions, while the series over the integers r in Eq. (52) simply reflects the angular character of the η variable, and is thus irrelevant. By the substitution of Eq. (52) back to Eq. (48) we obtain the energy spectrum for the finite volume theory:

$$E_l \equiv F(\rho=M=0, \eta=\langle \eta \rangle_l) = -E \cos \langle \eta \rangle_l = -E \cos \left(-\frac{q}{p} \theta + \frac{2\pi}{p} l \right). \quad (53)$$

Thus, we have found that the improved effective potential (48) has not one, but rather p physically different local extrema, when we look at the theory in the finite volume. The fact that the states (52) have different energies for generic values of θ is very important. This is where we find an essential difference of nonsupersymmetric gluodynamics from its supersymmetric extension. In the latter case, there are N_c degenerate states which all survive the infinite volume limit, and correspond to the physical Z_{2N_c} symmetry of SUSY YM theory [8,9,26]. The absence of degeneracy between the states (52) is therefore very natural, as there are no discrete symmetries for nonsupersymmetric gluodynamics in the thermodynamic limit $V \rightarrow \infty$ where we should stay along with just one true vacuum. Yet, as we will see in a moment, retaining the whole set of local extrema (52) is important to recover the correct periodicity in θ in the limit $V \rightarrow \infty$.

The remarkable fact about the extrema (52) is that they are related to each other by a cyclic permutation under the shift $\theta \rightarrow \theta + 2\pi$. The physics is perfectly periodic in θ with period 2π , as the minima $\langle \eta \rangle_l$, interchanging under the shift

⁹Note a remarkable similarity between Eq. (51) and the equation $\mu_i^2 \sin \phi_i = (a/N)(\theta - \Sigma \phi_j)$ (where μ_i and ϕ_i are the masses and phases of goldstone fields, respectively), obtained by Witten [16] as a minimization condition for the effective chiral Lagrangian for QCD. The limit $\varepsilon \rightarrow 0$ in Eq. (51) is analogous to the chiral limit $\mu_i^2 \rightarrow 0$ in this equation.

$\theta \rightarrow \theta + 2\pi$, can be just relabeled without altering anything. One of the minima always has a lowest energy. For example, if $0 \leq \theta < \pi/q$, it is the $l=0$ solution in Eq. (52). At the same time, we observe level crossing with a two-fold degeneracy at certain values of θ . One series of the level crossing points is given by $\theta = \pi \pmod{2\pi}$, irrespective of the values of the integers p, q . For example, at the first point $\theta = \pi$ in this series, the $l=0$ and $l=q$ solutions have the same energy $-E \cos(\pi q/p)$. This is the same series of level crossing points as was found for the Schwinger model. The difference from the Schwinger model is that now these values of θ do not correspond to level crossing of *lowest energy* states among the set (52). Instead, this happens for another series of level crossing points in θ , which is different from the previous one as long as $q \neq 1$. As can be seen from Eq. (53), it is the points $\theta_k = (2k+1)\pi/q$, $k=0,1,\dots,p-1$ where the lowest energy state is changing from the k th to the $(k+1)$ th branch in the set (52).

Let us now see what happens when the thermodynamic limit $V \rightarrow \infty$ is taken. The key observation is that a lowest energy state, which is the only one that should be retained in the limit $V \rightarrow \infty$ according to our convention (2), corresponds to different minima from the set (52), depending on an interval of variation of the vacuum θ angle. Thus, to perform the thermodynamic limit, we should first fix an interval of θ (say, $0 \leq \theta < \pi/q$), and only then select the state of lowest energy among the set (52). This solution will be the one corresponding to the single vacuum state in the limit $V \rightarrow \infty$, for all values of θ from this interval. This procedure can be described by the formula

$$F_{min} = -\lim_{V \rightarrow \infty} \frac{1}{V} \log \left\{ \frac{\sum_l \exp \left[VE \cos \left(-\frac{q}{p} \theta + \frac{2\pi}{p} l \right) \right]}{1 + \delta_{\theta - \pi/q, 0}} \right\}, \quad l=0,1,\dots,p-1 \quad (54)$$

[here $\delta_{\theta - \pi/q, 0}$ is the Kronecker symbol, equal to 1 if $\theta = (2k+1)\pi/q$ or 0 otherwise]. The multiplier $1/(1 + \delta_{\theta - \pi/q, 0})$ accounts for the two-fold vacuum degeneracy at the points $\theta = (2k+1)\pi/q$, $k=0,1,\dots,p-1$. We note that Eq. (54) is perfectly periodic in θ with period 2π .

Equation (54) shows that in the limit $V \rightarrow \infty$ cusp singularities occur at the values $\theta = (2k+1)\pi/q$, where the lowest energy vacuum state switches from one analytic branch to another one, much as it occurs in the Schwinger model. One should note that there is no physical jump at $\theta = \pi/q$. It is rather relabeling of a lowest energy state. The first derivative of the vacuum energy, which is proportional to the topological density condensate, is two-valued at these points. This means that whenever $\theta = (2k+1)\pi/q$, we stay with two degenerate vacua in the thermodynamic limit (Dashen phenomenon [18], see below). This picture of the singularity structure in θ resembles the one found for the lattice Z_p model in 4D [30].

If, on the other hand, the thermodynamic limit is performed for a fixed value of θ , any information on other states is completely lost in Eq. (54). Correspondingly, the 2π pe-

riodicity in θ is also lost in infinite volume formulas. We have no chance to know about additional states when we work in the infinite volume limit from the very beginning. As a result, usual $V=\infty$ formulas become blind to the very existence of a whole set of different vacua, which is just responsible for restoration of the 2π periodicity in θ . Instead, formulas corresponding to the formal limit $V=\infty$ look as suggesting a “wrong” (different from 2π) periodicity in θ ; see, e.g., Eqs. (20),(21). Now we know that this procedure of the shift $\theta \rightarrow \theta + 2\pi$ in the $V=\infty$ formulas is simply misleading as it is equivalent to going along a single analytic solution of the minimization equation (51), which does not correspond to a lowest energy state for a shifted value of θ . Comparing Eqs. (20) and (53), we see that the former may well describe the θ dependence in the physical limit $V \rightarrow \infty$ for small values $\theta < \pi/q$. To this end, we should set the ratio q/p , which so far was arbitrary, to the value $q/p = 2\xi$ (and take $E = -E_v$). At the same time, analyticity in θ of each separate branch (53) shows that the procedure of a formal resummation of the infinite Taylor series for small $\theta < \pi/q$, which has led to Eq. (20) [24], is legitimate. We therefore conclude that Eq. (20), which should be understood as standing for $\theta < \pi/q$, is not in conflict with general principles of periodicity and analyticity in θ for any rational value of the parameter ξ , including both particular choices $\xi = 2/b$ [23] or $\xi = 4/(3b)$ [24].

Although the problem of fixing the correct value of the parameter ξ is beyond the scope of this paper, we cannot refrain from pausing for a few comments on these matters.¹⁰ The parameter ξ is related to a number of different sectors of the theory, which are disconnected due to the superselection rule. One could think that this number of sectors is proportional to b , as the formulas $\xi = 4/(3b)$ [24] or $\xi = 2/b$ [23] suggest. However, the analysis of SUSY theories shows that it might not literally be the case. If in SQCD we change a number of flavors N_f keeping a number of colors N_c unchanged, the number of sector remains the same and strictly equals N_c (and not just proportional to N_c), though the β function $b \sim 3N_c - N_f$ changes. As a result, the angle θ enters physics in the combination θ/N_c for arbitrary N_f . Another argument comes from the analysis of softly broken SUSY gluodynamics where the gluino is given a small mass m . As discussed by Shifman [26], the situation is under control as long as m is small, and the number of different sectors remains the same N_c (though the degeneracy between them is lifted). On the other hand, the case of pure YM theory corresponds to the limit $m \rightarrow \infty$ (which means physically $m \gg \Lambda$). If the number of sectors N_c for small m does not discontinuously change when m becomes large, $m = \Lambda$, we end up with N_c different sectors for usual YM theory.

To summarize, different lines of reasoning lead to different values of ξ (though they all imply $\xi \sim N_c^{-1}$), and correspondingly to different values for a number of sectors in pure YM theory. However, irrespective of this particular number

(we only assume it be a rational), we know that there is only one true vacuum in the thermodynamic limit $V \rightarrow \infty$ and that the period of the θ dependence is always 2π .

After this digression we wish to discuss relations for the topological density condensate. Namely, we would like to see whether Eq. (21), obtained by a direct evaluation of correlation functions in YM theory, is consistent with results of this section. It is easy to see that it is indeed the case. Differentiating Eq. (53) in respect to θ , we obtain

$$-\frac{\partial E_l}{\partial \theta} = \frac{q}{p} E \sin\left(-\frac{q}{p}\theta + \frac{2\pi}{p}l\right). \quad (55)$$

As only the $l=0$ term survives the $V \rightarrow \infty$ limit for $0 \leq \theta < \pi/q$, we obtain, in agreement with Eq. (21)

$$\frac{1}{32\pi^2} \langle G\tilde{G} \rangle = -\frac{q}{p} E \sin\left(\frac{q}{p}\theta\right). \quad (56)$$

Similarly to what occurs in the Schwinger model, for the special case $\theta = \pi/q$ we stay in the limit $V \rightarrow \infty$ with two degenerate vacua which are distinguished by the sign of the topological density condensate:

$$\begin{aligned} |1\rangle &\equiv \left| \eta_{l=0} = -\frac{\pi}{p} \right\rangle, & \frac{1}{32\pi^2} \langle G\tilde{G} \rangle_1 &= -\frac{q}{p} E \sin\left(\frac{\pi}{p}\right), \\ |2\rangle &\equiv \left| \eta_{l=1} = \frac{\pi}{p} \right\rangle, & \frac{1}{32\pi^2} \langle G\tilde{G} \rangle_2 &= +\frac{q}{p} E \sin\left(\frac{\pi}{p}\right). \end{aligned} \quad (57)$$

As a CP transformation reverses the sign of θ , it exchanges the vacua $|1\rangle$ and $|2\rangle$: $CP|1\rangle = |2\rangle$, $CP|2\rangle = |1\rangle$. Therefore, the CP symmetry is broken at $\theta = \pi/q$. A similar phenomenon of vacuum doubling occurs for any point of the form $\theta_k = k\pi/q$, $k = 1, 2, 3, \dots$. For example, the $l=0$ and $l=q$ states are analogously related by a CP transformation at $\theta = \pi$. The reason we concentrate on the level crossing point $\theta = \pi/q$ is that at this value of θ the true vacuum (lowest energy state) switches from the $l=0$ to the $l=1$ branch, while at $\theta = \pi$ some excited states cross in energy. Therefore, in the sense of the lowest energy state among the set (52), the value $\theta = \pi$ corresponds to a regular, CP conserving point.

Finally, we would like to briefly describe the case of YM theory with an arbitrary (orthogonal, exceptional, etc.) gauge group G instead of the unitary $SU(N)$ that was discussed so far. For such a gauge group the second Casimir constant $C_2(G)$ and the β function would be different. Therefore, the only difference from the previous analysis in this case would be different values of the integers p and q , while the pattern of θ dependence would remain the same. Thus, the mechanism suggested in this paper seems to be valid for any gauge group.

¹⁰The arguments discussed below are due to Vainshtein [31], to whom we are indebted for sharing with us his insight.

VI. CONCLUSIONS

The most important results of the present analysis are the following.

(1) We have demonstrated that physics is periodic in θ with period 2π for an arbitrary gauge group. This behavior follows from our definition of the partition function for both the original and effective Lagrangian formulations of the theory, where the summation over all branches of a multivalued action is imposed. In the effective Lagrangian framework, this prescription is necessary for a single-valuedness and boundness from below of an effective potential.

(2) The periodicity in θ with period 2π is perfectly compatible with the θ/N dependence found in a number of models at small θ . The correct periodicity in θ is recovered when a whole set of different branches is taken into account. The standard definition of the thermodynamic limit selects only a lowest energy state among this set. As a result, the thermodynamic limit and the shift $\theta \rightarrow \theta + 2\pi$ do not commute (in the sense explained in the Introduction).

(3) For generic values of θ , there is one and only one vacuum state in the thermodynamic limit. For $\theta = \pi/q$ there are exactly two degenerate states, which are distinguished by the sign of the topological density condensate.

We would like to end up with some speculations. We emphasize again that $\theta = \pi/q$ is a very special point because of the vacuum degeneracy which does not follow from any obvious symmetry of the original Lagrangian. This degeneracy may imply the existence of domain walls in the theory at $\theta = \pi/q$, which are static field configurations depending only on one spatial coordinate. An effective potential describing domain walls could be obtained from Eq. (48) by freezing the ρ and M fields. Such a potential is a complicated function of the η field which, however, reduces to the standard Sine-Gordon form near the points (52); see Eq. (53). Provided a kinetic term (we recall that kinetic terms are not fixed by the Ward identities) is added, the theory could sustain domain wall configurations. The existence of these solutions in gauge theories could have interesting consequences for cosmology and particle physics.

We would also like to speculate that the above “ p ” non-equivalent states, could be really observed in some nonequilibrium high energy processes with a finite geometry, where the superselection rule cannot be applied (a similar comment was made by Shifman [26]). Such a situation could be realized, e.g., in nuclear-nuclear collisions, where the appearance of droplets of a “false vacuum” would be similar to the production of droplets of disoriented chiral condensate, see e.g. [32] for a review. Instead of an arbitrary direction of the chiral condensate for the latter, in the former case we would deal with “ p ” different values of the topological density condensate $\langle G\tilde{G} \rangle$. One expects that this phenomenon, if it exists, should be related to the physics of the η' meson and CP violation. Yet, it is not known at the moment how to formulate this problem in an appropriate way.

The inclusion of the light quarks into the effective Lagrangian framework and the resulting picture of the θ dependence in QCD will be discussed in [33].

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APPENDIX

The purpose of this appendix is to discuss in somewhat more detail the derivation of the low energy theorems (16) and (19) and, in particular, a procedure of ultraviolet regularization which was implied in Eqs. (16) and (19). We start with the Novikov-Shifman-Vainshtein-Zakharov (NSVZ) low energy theorem [23], Eq. (16), which is here repeated for convenience:

$$\begin{aligned} \lim_{q \rightarrow 0} i \int dx e^{iqx} \langle 0 | T \left\{ \frac{\beta(\alpha_s)}{4\alpha_s} G^2(x) \frac{\beta(\alpha_s)}{4\alpha_s} G^2(0) \right\} | 0 \rangle \\ = -4 \left\langle \frac{\beta(\alpha_s)}{4\alpha_s} G^2 \right\rangle, \end{aligned} \quad (\text{A1})$$

where $\beta(\alpha_s) = -b\alpha_s^2/(2\pi) + O(\alpha_s^3)$ is the Gell-Mann–Low β function for YM theory with $b = (11/3)N_c$, and N_c is the number of colors.

The low energy theorem was obtained in [23] using the one-loop β function with a particular attention to a regularization of ultraviolet (UV) divergences, arising in the two-point function (A1), within Pauli-Villars procedure. In this derivation Dyson type of the T-product symbol was implied in Eq. (A1). It was shown that quadratically divergent UV contributions cancel out identically in both sides of Eq. (A1). This implies that perturbative contributions should always be subtracted in vacuum condensates such as $\langle \beta(\alpha_s)/(4\alpha_s)G^2 \rangle$ in Eq. (A1). Once this rule is accepted, the dependence of any (nonperturbative) condensate $\langle O \rangle_{NP}$ of dimension d on the bare coupling constant g_0 (normalized at the cut-off scale M_R) is fixed by the dimensional transmutation formula:

$$\langle O \rangle_{NP} = \text{const} \times \left[M_R \exp \left(-\frac{8\pi^2}{bg_0^2} \right) \right]^d, \quad (\text{A2})$$

and the derivation of the NSVZ theorem proceeds as described in Sec. III, where the path integral definition of correlation functions is used. The latter implies Wick type of the T-product symbol. This definition of zero momentum correlation functions (18) automatically ensures the same type of renormalization for all such functions, which is fixed by a rule of subtracting perturbative UV divergent contributions to the conformal anomaly (with, e.g., Pauli-Villars regularization). The latter procedure thus defines a nonperturbative gluon condensate in the θ vacuum $\langle g^2 G^2 \rangle_\theta$, i.e. a nonperturbative part of the conformal anomaly calculated for given θ . Its dependence on $1/g_0^2$ is given by Eq. (A2). Zero momentum correlation functions of the operator $g^2 G^2$ are ob-

tained by the differentiation of the nonperturbative part of the partition function $\log(Z/Z_{PT})$ (Z_{PT} stands for a perturbatively defined partition function which does not depend on θ), where

$$\begin{aligned} Z(\theta) &= Z_{PT} \exp\{-iVE_v(\theta)\} \\ &= Z_{PT} \exp\left\{-iV\langle 0| -\frac{b\alpha_s}{32\pi} G^2|0\rangle_\theta\right\}, \end{aligned} \quad (\text{A3})$$

in respect to $1/g_0^2$. Note that the factor $\partial \log Z_{PT}/\partial(g_0^{-2})$ corresponds to the correlation function (A1) in perturbation theory.

It is a subtraction of perturbative contributions in vacuum condensates (A2) that we here would like to comment upon. Technically, this prescription can be thought of as the requirement of absence of regular powers of the coupling constant α_s in vacuum condensates $\langle O \rangle_{NP}$ to any finite order in α_s . For two-dimensional models, it has been shown [34] that the definition of vacuum condensates via the path integral automatically nullifies perturbative contributions to the condensates. Moreover, this procedure gives results identical to a point-splitting regularization with Dyson type of the T product. One can notice that in four dimensions the separation of genuinely perturbative and nonperturbative contributions to physical quantities is ambiguous as it depends on a definition of the sum of perturbative series. Still, there is nothing wrong with the requirement that the ‘‘nonperturbative’’ condensates contain the coupling constant g_0^2 as in Eq. (A2), while the regular powers of g_0^2 are absent. The difference between different regularization schemes is reduced in this case to possible finite renormalizations (different numerical values) of the vacuum condensates. Such a choice of the nonperturbative gluon condensate in Eq. (A3) is the only ambiguity for all multipoint correlation functions (18).

Next we would like to discuss zero momentum correlation functions of the topological density operator. With Wick definition of the T product we obtain from Eq. (A3)

$$\begin{aligned} \lim_{q \rightarrow 0} \int dx e^{iqx} \langle 0| T \left\{ \frac{\alpha_s}{8\pi} G\tilde{G}(x) \frac{\alpha_s}{8\pi} G\tilde{G}(0) \right\} |0\rangle & \\ = -\frac{\partial^2 E_v(\theta)}{\partial \theta^2} = -\frac{1}{4} \frac{\partial^2}{\partial \theta^2} \langle \sigma \rangle_\theta. \end{aligned} \quad (\text{A4})$$

[Equation (A4) is written for Minkowsky space, and σ stands for the trace of the energy-momentum tensor.] A few comments on Eq. (A4) are in order. We note that the two definitions (through Dyson or Wick T products) are equivalent for the correlation function (A1). For correlation functions of the topological density Q , this is no longer the case. Witten-Veneziano construction [5] specifically implies [35,36] Wick T product in the two-point function (A4). This can be seen both from the definition of zero momentum correlation functions of the operator Q used in [5], and from the fact the a gauge non-invariant axial ghost (Veneziano ghost pole) cannot appear in Dyson T product which is related to contributions of intermediate gauge-invariant states only.

This is why Wick type of the T product was used in Eq. (A4). With this definition the two-point function (A4) does not contain UV divergences which are present in Z_{PT} and drop out after the differentiating of $\log Z$ in respect to θ . We note that an attempt to calculate the correlation function (A4) using Dyson T product (and adding corresponding contact terms) would face a problem due to the fact that, in contrast to the trace of the energy-momentum tensor, the topological density operator in pure YM theory is not seen [37] to be related to any quantity conserved at the classical level. Therefore, the canonical methods with Pauli-Villars regularization procedure used in [23] would apparently be not applicable in this case.

We further require that the θ dependence in Eq. (A3) is described by a single dimensionless function $f(\theta)$ such that

$$\frac{\partial^2}{\partial \theta^2} \langle \sigma \rangle_\theta = \frac{\partial^2}{\partial \theta^2} (\langle \sigma \rangle_0 f(\theta)) = \langle \sigma \rangle_0 f''(\theta). \quad (\text{A5})$$

Any other form of introducing the θ dependence can be reduced to Eq. (A5). For example, the ansatz $\langle \sigma \rangle_\theta = \langle \sigma \rangle_0 f_1(\theta) + \Lambda_{YM}^4 f_2(\theta)$ could be transformed to the form (A5) by the redefinition $f_1(\theta) + f_2(\theta) \Lambda_{YM}^4 / \langle \sigma \rangle_0 \rightarrow f(\theta)$. A function $f(\theta)$ should satisfy the constraints $f(0)=1$, $f'(0)=0$, which means that its small θ expansion reads

$$f(\theta) = 1 - 2\xi^2 \theta^2 + \dots, \quad (\text{A6})$$

where ξ^2 is some dimensionless number. Using this in Eq. (A4), we obtain

$$\begin{aligned} \lim_{q \rightarrow 0} \int dx e^{iqx} \langle 0| T \left\{ \frac{\alpha_s}{8\pi} G\tilde{G}(x) \frac{\alpha_s}{8\pi} G\tilde{G}(0) \right\} |0\rangle_{\theta=0} & \\ = \xi^2 \left\langle -\frac{b\alpha_s}{8\pi} G^2 \right\rangle_{\theta=0}. \end{aligned} \quad (\text{A7})$$

The assumption made in Eq. (19) in the text was that Eq. (A7) is covariant in θ , i.e., remains of the same form (A7) not only for $\theta=0$, but also for small values $\theta \neq 0$. This requirement fixes the function $f(\theta)$ completely:

$$f''(\theta) = -4\xi^2 f(\theta) \Rightarrow f(\theta) = \cos(2\xi\theta), \quad (\text{A8})$$

which results in the θ dependence of the vacuum energy and topological density condensate identical to the one displayed in Eqs. (20) and (21). This assumption is self-consistent because the same Eqs. (20),(21) can be obtained without fixing the function $f(\theta)$, but instead by postulating the covariant relation (19) and resumming Taylor expansions in θ for the condensates $\langle G^2 \rangle_\theta, \langle G\tilde{G} \rangle_\theta$, as was done in [24]. One more relation needed for this purpose reads

$$i \int dx \langle 0 | T \left\{ \frac{\alpha_s}{8\pi} G^2(x) \frac{\alpha_s}{8\pi} G \tilde{G}(0) \right\} | 0 \rangle = \frac{4}{b} \left\langle \frac{\alpha_s}{8\pi} G \tilde{G} \right\rangle, \quad (\text{A9})$$

which is a particular version of the original NSVZ theorem [23]. Equation (A9) is valid for any small θ .

Any other choice for the function $f(\theta)$, different from Eq. (A8), would presumably not be self-consistent, though we did not find a general proof of this statement. One should stress that the form (A8), implying the reiteration of the parameter ξ^2 in multipoint correlation functions of the operator Q , is consistent with Veneziano construction [5] for the ghost pole mechanism, where it was found that

$$\frac{\partial^{2n-1}}{\partial \theta^{2n-1}} \langle Q \rangle |_{\theta=0} \sim (-1)^{n-1} N_c \left(\frac{\lambda}{N_c} \right)^{2n-1},$$

$$N_c \rightarrow \infty, \quad \lambda = O(N_c^0). \quad (\text{A10})$$

At the same time, Eq. (A8) relates the ghost pole residue in Veneziano scheme with conformal anomaly in the theory with $\theta \neq 0$, in terms of the parameters $\xi, \langle \sigma \rangle_0$. In our work [24], a particular choice, $\xi = 4/(3b)$, was advocated using a one-loop connection between the conformal and axial anomalies in the theory with an auxiliary heavy fermion. Moreover, the covariance of Eq. (A7) in respect to θ followed automatically within a procedure used in [24], where Eq. (A7) with $\xi = 4/(3b)$ was obtained directly from the NSVZ relation (A1) which is valid for any small θ .

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