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The $U_A(1)$ Problem on the Lattice with Ginsparg-Wilson Fermions

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ABSTRACT

We show how it is possible to give a precise and unambiguous implementation of the Witten–Veneziano formula for the η' mass on the lattice, which looks like the formal continuum one, if the expression of the topological charge density operator, suggested by fermions obeying the Ginsparg–Wilson relation, is employed. By using recent numerical results from simulations with overlap fermions in 2 (abelian Schwinger model) and 4 (QCD) dimensions, one obtains values for the mass of the lightest pseudo-scalar flavour-singlet state that agree within errors with theoretical expectations and experimental data, respectively.

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1 Introduction

Lacking any reliable analytical way to compute bound-states masses in a strongly interacting theory, a crucial confirmation of QCD as the theory of hadron dynamics has come in recent years from our ability to compute from first principles the masses of the lightest hadrons in Lattice QCD (LQCD) [1]. This has been done with remarkable success for a number of mesonic and baryonic states, both in the quenched approximation (no fermion determinant) and, more recently, also in the full (unquenched) theory [2].

A somewhat difficult problem is, computationally, the inclusion of diagrams violating the so-called OZI-rule [3], i.e. of diagrams involving purely gluonic intermediate states: these require the calculation of the trace of the inverse Dirac operator, and are affected by large statistical fluctuations. The very existence of such diagrams is a key property of QCD, making it differ in an essential way from any naive quark model. Since OZI-violating diagrams are the ones that distinguish flavour-singlet from flavour-non-singlet states, their inclusion in LQCD is crucial and should allow for the theoretical computation of subtle phenomena, such as $\rho - \omega - \phi$ and $\pi - \eta - \eta'$ splitting and mixing. In fact, one of the most striking experimental facts in hadronic physics is the contrast between the vector (as well as the tensor) mesons, that appear to satisfy the OZI-rule to high accuracy, and the pseudo-scalar mesons, whose $(\text{mass})^2$ eigenstates are very far from being ideally mixed (the OZI-prediction), and whose eigenvalues exhibit a peculiar hierarchical structure, $m_\pi^2 \ll m_\eta^2 \ll m_{\eta'}^2$.

The technical problems mentioned above have so far prevented in LQCD a fully-fledged evaluation of the η' mass at the same level of accuracy as that reached for the other light hadrons, although noticeable progress has been recently made in this direction [4, 5].

In quenched LQCD the first evaluation of the η' mass [2] dates back to the work of ref. [6], where the OZI-violating (ZV) and the OZI-conserving (ZC)

[2]Throughout this paper we will indicate by η' the flavour-singlet pseudo-scalar meson, ignoring vector flavour symmetry-breaking effects. We will work in Euclidean metric with hermitian γ matrices satisfying $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$ and $\mathrm{tr}(\gamma_5\gamma_1\gamma_2\gamma_3\gamma_4) = 4\epsilon_{1234} = 4$. Left-handed and right-handed fermions are defined through the equations $\gamma_5\psi_L = \psi_L$ and $\gamma_5\psi_R = -\psi_R$, respectively. Colour generators, T^a $(a = 1, ..., N_c^2 - 1)$, in the fundamental representation are normalized according to $\mathrm{tr}(T^a T^b) = \delta^{ab}/2$.

contributions to the 2-point meson–meson Green function

$$\Gamma_q(t) = \int d\vec{x}\, \langle P^0(\vec{x},t) P^0(0)\rangle\Big|_{\text{quenched}} \tag{1}$$

were computed. In eq. (1)

$$P^0 = \sum_{r=1}^{N_f} \bar{\psi}^r \gamma_5 \psi_r \tag{2}$$

is the pseudo-scalar singlet quark density, with N_f the number of light quarks. The (quenched value of the) η' mass is identified as the amount by which the singlet pseudo-scalar $\bar{q}q$-boson pole gets shifted owing to the iteration of Nambu–Goldstone (NG) particle exchanges, the sum of which builds up the full (unquenched) expression of Γ. This leads to the formula

$$m^2_{\eta'} = 2m_\pi \lim_{t\to\infty} \frac{\Gamma_q^{\mathrm{ZV}}(t)}{|t|\Gamma_q^{\mathrm{ZC}}(t)}\,. \tag{3}$$

Numerical data were encouraging, but far from convincing. Although considerable progress has been achieved along these lines in more recent simulations [7, 8], in our opinion one cannot regard the present numerical results as really conclusive.

From a more theoretical point of view, leaving aside the lattice for a moment, the striking difference between vector and pseudo-scalar mesons appeared as a serious problem within the generally accepted framework according to which the light pseudo-scalar mesons are the (quasi) NG bosons of a spontaneously (and also explicitly) broken chiral symmetry. As first noted by Glashow [9], a naive use of spontaneously-broken chiral symmetry calls for nine - rather than eight - light NG bosons ($N_f = 3$). Thus one would naively expect that chiral symmetry should "protect" the OZI-rule in the pseudo-scalar channel, while the opposite is experimentally true.

Awareness of the problem was reinforced by a very influential paper by Weinberg [10] in which, under what he calls "plausible assumptions", the bound

$$m_{\mathrm{octet},I=0} < \sqrt{3}m_\pi \tag{4}$$

was derived in the absence of $U_A(1)$ anomaly contributions.

Since the very beginning, the famous ABJ anomaly [11] was suspected to have much to do with the resolution of the $U_A(1)$ puzzle, as the strong

(QCD) axial anomaly appears only in the flavour-singlet channel. But the fact that the anomaly itself is a total divergence (albeit of a non-gauge-invariant current) made it look irrelevant for the solution of the problem. Kogut and Susskind [12] were the first to notice that the ABJ anomaly could be made effective again, if one assumed the existence of a "ghost" particle, a massless state coupled to the non-gauge-invariant current, but decoupled from any gauge-invariant operator.

Things took a decisive turn when, in 1976, 't Hooft [13] pointed out that the resolution of the $U_A(1)$ problem had to be related to the existence of topologically non-trivial gauge field configurations (instantons) in Euclidean QCD. Soon after, Crewther [14] emphasized that 't Hooft's crucial observation could only be considered a solution of the problem, if it could pass a number of theoretical tests, in particular that of satisfying both the conventional (i.e. non-anomalous) and anomalous Ward–Takahashi Identities (WTI's). Several puzzles, related to the dependence on the number and masses of quark flavours appeared, in fact, to be still present [14].

Fortunately, these questions can be addressed and solved by exploiting the simplifications that occur in certain limits of QCD. One such limit, employed in ref. [15], is the 't Hooft limit ($N_c \to \infty$, with $g^2 N_c$ and N_f held fixed [16]). The other possibility, proposed in ref. [17], proceeds by assuming that anomalous flavour-singlet axial WTIs retain their validity order by order in an expansion in $u \equiv N_f/N_c$ around $u = 0$ [3]. In either cases one can derive the leading-order Witten–Veneziano (WV) relation

$$m^2_{\eta'} = \frac{2N_f}{F_\pi^2} A \,, \tag{5}$$

where $F_\pi \simeq 94\,\mathrm{MeV}$ is the pion decay constant and A is the "topological susceptibility". A is formally defined by the equation

$$A = \int d^4x \, \langle Q(x) Q(0) \rangle \Big|_{\mathrm{YM}} \,, \tag{6}$$

where $Q(x)$ is the topological charge density

$$Q(x) = \frac{g^2}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \mathrm{tr}[F_{\mu\nu} F_{\rho\sigma}(x)] \tag{7}$$

[3]This expansion is not to be confused with the topological expansion ($N_c \to \infty$ at fixed $g^2 N_c$ and u), introduced in ref. [18].

and the trace is over colour indices. The notation $\langle ...\rangle|_{\mathrm{YM}}$ in eq. (6) means that the QQ-correlation function is to be computed in the pure Yang–Mills (YM) theory, i.e. in the absence of quarks.

We recall that, within the approach of ref. [15], eq. (5) is expected to be valid for large N_c, while, relying on the derivation given in ref. [17], one would conclude that the η' mass formula is valid for any value of N_c at leading order in u. We also notice that the limit $u \to 0$ at fixed $g^2 N_c$ encompasses the 't Hooft limit ($N_c \to \infty$ at fixed N_f) and that the equivalence of eqs. (3) and (5) essentially relies on the validity of anomalous flavour-singlet WTIs order by order in u [17].

Since the pioneering works of refs. [13], [15] and [17], a large number of papers (see, for instance, [19]–[25] and references therein) have appeared, aimed at checking the validity of eq. (5) by comparing the number obtained by inserting in it the value of A extracted from pure gauge lattice simulations with the experimental magnitude of the η' mass [4].

The formal eqs. (5) and (6), when translated in any regularized version of QCD, such as LQCD to which we will refer in the following, become more complicated and quite a number of subtleties have to be dealt with in order to be able to determine the correct field theoretical expression of A, which should be inserted in the η' mass formula.

Two main problems need to be solved to make eqs. (5) and (6) rigorous and of practical use. One has to i) find a properly normalized lattice definition of the topological charge density Q_L; ii) subtract from the $Q_L(x)Q_L(0)$ operator product appropriate contact terms, as required to make it an integrable (operator-valued) distribution.

Three types of prescriptions have been proposed upon addressing the first problem. They can be succinctly described as follows.

- Take any naive lattice discretization of $F_{\mu\nu}$ [19] [27] [28] and construct Q_L through (the lattice version of) eq. (7) by properly normalizing it [22].

- Define Q_L by making reference to the anomalous flavour-singlet axial WTIs [29] [23] [30].

[4] The question of how eq. (5) should be modified beyond the chiral limit was addressed in refs. [17, 26].

- Exploit the topological nature of Q to give a definition of it appropriate to a discrete manifold [31].

The second problem is actually more subtle than stated above. In fact, it is not sufficient to subtract (possible) *divergent* contact terms from the r.h.s. of eq. (6), by taking properly into account the mixing of $Q(x)Q(0)$ with lower dimensional operators. It is also necessary to fix *finite* contact terms of the form, say, $c\,\delta(x)$, since, as also stressed in ref. [14], they would contribute a constant to the η' mass when inserted in eq. (6).

The question of the subtraction of lower dimensional operators was addressed in an incomplete way and in perturbation theory in ref. [19], and in a more refined, non-perturbative, way in ref. [22]. The issue was taken up again more recently within the overlap formulation of LQCD [32, 30] (see ref. [33] for a recent review).

The purpose of this paper is to give a rigorous derivation of a formula for the η' mass, which could be unambiguously used in numerical simulations. The validity of such a formula is a crucial test of QCD, as it directly relates the non-vanishing of the η' mass in the chiral limit to the explicit breaking of the $U_A(1)$ symmetry induced at the quantum level by the gluon anomaly.

Our strategy is to use (lattice) regularized anomalous flavour-singlet axial WTIs of full QCD in order to properly construct the $\langle QQ\rangle$ correlation function, as a well defined (integrable) distribution. The remarkable result of our analysis is that no subtraction is needed to this end in the chiral limit, if the definition of lattice topological charge density suggested by fermions obeying the Ginsparg–Wilson (GW) relation [34] (e.g. overlap fermions [32, 30]) is employed. In this case a formula for the η' mass, which looks like the naive continuum one (i.e. which closely parallels the structure of eqs. (5) and (6)), can be obtained.

The case of Wilson fermions is somewhat more involved and will be discussed in a forthcoming publication [35].

The paper is organized as follows. In sect. 2 we recall the derivation of the η' mass formula in the continuum. In sect. 3 we show how one can give a precise meaning to this relation in the QCD regularization offered by GW fermions. In sect. 4 we discuss the numerical evidence in favour of the WV formula in 2 and 4 dimensions, which emerges from the existing overlap fermion simulation data. Conclusions can be found in sect. 5. In an Appendix we derive several relations between unquenched and quenched QCD quantities, involving moments of the topological susceptibility, including the WV formula.

2 The η' mass formula in the continuum

In this section we review the formal derivation of the WV formula in the continuum. We start from the anomalous flavour-singlet WTI

$$\partial_\mu \langle A^0_\mu(x) Q(0)\rangle = 2m_q \langle P^0(x) Q(0)\rangle + 2N_f \langle Q(x) Q(0)\rangle \,, \tag{8}$$

where

$$A^0_\mu = \sum_{r=1}^{N_f} \bar{\psi}^r \gamma_\mu \gamma_5 \psi_r \tag{9}$$

is the axial current, P^0 was defined in eq. (2), Q is the topological charge density and m_q is the quark mass. It is understood that all operators in eq. (8) are finite (i.e. have finite insertions with any string of renormalized fundamental fields), so that every term in eq. (9) is finite as soon as $x \neq 0$.

The Fourier transform of eq. (8) in the chiral limit reads

$$\begin{aligned} & ip_\mu \int d^4x \, \mathrm{e}^{-ipx} \langle A^0_\mu(x) Q(0)\rangle + \mathrm{CT}(p) = \\ & = 2N_f \int d^4x \, \mathrm{e}^{-ipx} \langle Q(x) Q(0)\rangle + \mathrm{CT}(p) \equiv 2N_f \chi_t(p) \,. \end{aligned} \tag{10}$$

A contact term, $\mathrm{CT}(p)$, has been added to both sides of eq. (10) to make them separately finite. $\mathrm{CT}(p)$ is a polynomial of degree 4 in p, which vanishes at $p = 0$, because the Fourier transform of the l.h.s. of eq. (8) is certainly finite (actually zero) at $p = 0$ in the full theory. As will become clear in the following, $\mathrm{CT}(p)$ plays no rôle in the main line of arguments we present in this paper, since finally we will be only interested in the value of χ_t at $p = 0$ [5].

The absence of zero-mass particles in the pseudo-scalar singlet channel implies the "sum rule"

$$\chi_t(0) = 0 \,. \tag{11}$$

[5] The presence of $\mathrm{CT}(p)$ will, instead, affect the determination of quantities like $\chi'_t(0) = d\chi_t(p^2)/dp^2|_{p=0}$, unless $\mathrm{CT}(p) \propto p^4$ [36]. $\chi'_t(0)$ is relevant to the discussion of the so-called proton spin crisis problem [37]. We will elaborate further on this issue in the Appendix.

This relation is the famous statement that the topological susceptibility in full QCD vanishes in the chiral limit.

One can derive from it a formula for the η' mass whenever the topological susceptibility in the absence of quarks is non-zero. In this situation, in fact, the vanishing of $\chi_t(p)$ at $p=0$ in full QCD to any order in u, can possibly take place only if there exists a $\bar{q}q$-meson contributing to $\chi_t(p)$, whose mass goes to zero (linearly) as $u \to 0$ [15] [17]. Under these circumstances the limit $p \to 0$ and the expansion of $\chi_t(p)$ around $u=0$ do not commute. In the Appendix we give a derivation of the WV formula along these lines and prove a number of other interesting related equations. The formulae that are obtained are derived under the assumption that at $p \neq 0$ all the relevant quantities and correlators are smooth functions of u and, in particular, that taking the limit $u \to 0$ is equivalent to neglecting the fermion determinant. In the following, for short, we will refer to this assumption as the "smooth-quenching hypothesis".

To leading order in u one then obtains for the η' mass either the formula

$$m_{\eta'}^2 = \frac{1}{F_\pi^2} \int d^4x \, \partial^\mu \langle A_\mu^0(x) Q(0) \rangle \Big|_{\text{quenched}} \,, \tag{12}$$

or, equivalently

$$m_{\eta'}^2 = \frac{2N_f}{F_\pi^2} \int d^4x \, \langle Q(x) Q(0) \rangle \Big|_{\text{YM}} \,. \tag{13}$$

We stress that, under the above assumptions, the r.h.s. of (13) (as well as that of eq. (12)) is ultraviolet-finite, because $\mathrm{CT}(p)$ is a polynomial in p that vanishes at $p=0$ for any value of u.

In the next section we will show how it is possible to give a precise meaning to the above equations, starting with the chirally invariant regularization of QCD offered by fermions obeying the GW relation. In this framework we will be able to derive an unambiguous formula for the η' mass, immediately usable in actual Monte Carlo simulations.

We conclude by remarking that eq. (12) cannot be employed for direct numerical evaluations, because its r.h.s. is actually identically zero at finite volume, as there are no massless particles in a finite box. However, it can be put in a form that is amenable to numerical simulations, if one goes one step further and rewrites it in the form [6]

$$m^2_{\eta'} = \frac{\sqrt{2N_f}}{F_\pi} \langle 0|Q|\eta'\rangle\Big|_{\rm quenched} . \tag{14}$$

This equation follows from the fact that in the quenched limit the integral in the r.h.s. of eq. (12) is exactly given at the chiral point by the contribution of the pole of the singlet pseudo-scalar particle, as the mass of the latter vanishes in that limit. No explicit reference to the size of the volume in which the system is enclosed appears anymore in eq. (14). We will make use of these considerations in sect. 3.1.

3 Ginsparg-Wilson fermions

Regularizing the fermionic part of the QCD action using GW fermions [34, 32, 30] offers the great advantage over the standard Wilson discretization [1] that global chiral transformations can be defined, which are an exact symmetry of the massless theory, as in the formal continuum limit. This is a consequence of the relation [34] [7]

$$\gamma_5 D + D\gamma_5 = D\gamma_5 D \,, \tag{15}$$

obeyed by the GW Dirac operator, D. In this regularization the $U_A(1)$ anomaly is recovered à la Fujikawa [38], as a consequence of the non-trivial Jacobian that accompanies the change of fermionic integration variables induced by a $U_A(1)$ lattice transformation. In fact, it can be shown [39] that under the infinitesimal global transformations

$$\begin{aligned} \psi &= \psi' + \epsilon\gamma_5(1-D)\psi' \\ \bar\psi &= \bar\psi' + \epsilon\bar\psi'\gamma_5 \end{aligned} \tag{16}$$

the massless action, thanks to (15), remains invariant, while the functional integration measure gets multiplied by the factor

$$J = \exp\{\epsilon \int d^4x\, {\rm Tr}[\gamma_5 D(x,x)]\} \,, \tag{17}$$

[6] See the Appendix for the relevant normalizations and notations.

[7] We set the lattice spacing, a, equal to 1. It is, however, understood that in all lattice formulae the continuum limit should be finally taken.

where Tr is over colour and spin indices. In view of these results it is concluded that [8]

- the index theorem for the GW Dirac operator reads (for each flavour)

$$n_R - n_L = \mathrm{index}(D) = \frac{1}{2}\int d^4x\,\mathrm{Tr}[\gamma_5 D(x,x)]\,; \tag{18}$$

- for sufficiently smooth gauge configurations [42] one has

$$\frac{1}{2}\mathrm{Tr}[\gamma_5 D(x,x)] = \frac{g^2}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}[F_{\mu\nu}F_{\rho\sigma}(x)]\,; \tag{19}$$

- the anomalous flavour-singlet WTIs in the presence of N_f massless fermions take the form

$$0 = \frac{2N_f}{2}\int d^4x\,\langle \mathrm{Tr}[\gamma_5 D(x,x)]\hat{O}\rangle + \langle \delta_A \hat{O}\rangle\,, \tag{20}$$

  where $\hat{O}$ is any finite (multi)local operator. In eq. (20) we have symbolically indicated by $\epsilon\delta_A\hat{O}$ the infinitesimal variation of $\hat{O}$ under the transformations (16). Equation (20) assumes the absence of a $U_A(1)$ NG boson.

Starting with the local version of the transformations (16), one gets in the chiral limit the local WTIs

$$\nabla_\mu\langle A^0_\mu(x)\hat{O}\rangle = \frac{2N_f}{2}\langle \mathrm{Tr}[\gamma_5 D(x,x)]\hat{O}\rangle + \langle \delta^x_A \hat{O}\rangle\,, \tag{21}$$

where $\delta^x_A\hat{O}$ is the local variation of $\hat{O}$; $\nabla_\mu A^0_\mu(x)$ is the divergence of the singlet axial current, a quantity that formally vanishes when integrated over all space-time.

Neither $\mathrm{Tr}[\gamma_5 D(x,x)]$ nor $A^0_\mu(x)$ are finite operators, but finite linear combinations are easily constructed [43, 44]. In fact, since the second term in the r.h.s. of eq. (20) is obviously finite, if $\hat{O} \to \hat{\Lambda}_n \equiv \psi_R(x_1)...\bar{\psi}_R(x_n)$, it follows that the integrated operator $\int d^4x\,\mathrm{Tr}[\gamma_5 D(x,x)]$ is also finite, as it

[8] Actually the GW relation (15) alone may not be enough to ensure the validity of eqs. (18) and (19) below [40]. These equations are, however, valid if overlap fermions are used [41] and, more generally, if the admissibility condition of ref. [42] is fulfilled.

has finite insertions with any string of renormalized fundamental fields. This statement in turn implies that $\mathrm{Tr}[\gamma_5 D(x,x)]$ can only mix with operators of dimension ≤ 4 and vanishing integral, hence only with $\nabla_\mu A^0_\mu(x)$. Calling Z the relevant mixing coefficient, one can define the finite operators $\hat{Q}$ and $\hat{A}^0_\mu$ by writing

$$\hat{Q}(x) = \frac{1}{2}\mathrm{Tr}[\gamma_5 D(x,x)] - \frac{Z}{2N_f}\nabla_\mu A^0_\mu(x) \tag{22}$$

$$\hat{A}^0_\mu(x) = (1-Z)A^0_\mu(x)\,. \tag{23}$$

Z is logarithmically divergent to lowest order in perturbation theory and vanishes as $u \to 0$. Its perturbative expansion starts at order g^4.

With the above definitions the renormalized singlet axial WTI becomes

$$\nabla_\mu \langle \hat{A}^0_\mu(x)\hat{O}\rangle = 2N_f\langle \hat{Q}(x)\hat{O}\rangle + \langle \delta^x_A \hat{O}\rangle\,. \tag{24}$$

We expressly note that 1) as the comparison of the WTIs (21) and (24) shows, the operators $\hat{Q}$ and $\hat{A}^0_\mu$ are already correctly normalized, so no further (finite) multiplicative renormalization is required; 2) the line of arguments given above also proves that there is no mixing of $\mathrm{Tr}[\gamma_5 D(x,x)]$ with operators of dimension smaller than 4 (like the pseudo-scalar quark density), which would bring in dangerous power divergent mixing coefficients. This fact is related to the absence of power-like divergent, $1/a$, subtraction in the definition of renormalized quark mass. All these are very distinctive features of GW fermions which are at variance with what happens in the case of Wilson fermions [9].

3.1 The η' mass formula on the lattice

A formula for the η' mass can be easily obtained from the WTI (21), assuming that in the limit $u \to 0$ the η' mass is $\mathrm{O}(u)$. A more sophisticated derivation can be found in the Appendix.

One starts by defining the lattice Green function

$$\chi_{tL}(p) = \frac{1}{2N_f}\int d^4x\, \mathrm{e}^{-ipx}\nabla_\mu\langle \hat{A}^0_\mu(x)\hat{Q}(0)\rangle\,, \tag{25}$$

[9] We are indebted to M. Lüscher for pointing out to us the possible existence of mixing between Q and P^0 in the case of lattice Wilson fermions.

with $\hat{Q}$ given by eq. (22). The same observation, that was made in sect. 2 after eq. (10) about the presence of counter-terms necessary to make the correlator (25) finite at $p \neq 0$, applies also here. However, as this counter-term does not play any rôle in the determination of the η' mass, for brevity we will not indicate it explicitly in the formulae of this section.

In the full theory, where the η' is massive, one gets

$$\chi_{tL}(0) = 0\,, \tag{26}$$

which is the (lattice) regularized version of eq. (11).

The key observation at this point is that, at vanishing quark mass, in the limit $u \to 0$, only the η' pole contributes to $\chi_{tL}(p)$, as explained below eq. (14), giving (see eqs. (49) and (56) of the Appendix)

$$\lim_{p\to 0}\lim_{u\to 0}\chi_{tL}(p) = \frac{F_\pi^2}{2N_f} m_{\eta'}^2\Big|_{u=0}\,. \tag{27}$$

Recalling that $F_\pi = \mathrm{O}(\sqrt{N_c})$ [16, 18] to leading order in u, we see that consistently the combination in the r.h.s. of this equation has a finite limit as $u \to 0$.

On the other hand, using the WTI (21) with $\hat{O} = \hat{Q}$, we can put eq. (25) in the form

$$\begin{aligned}&\chi_{tL}(p) = \\ &= (1-Z)\int d^4x\, \mathrm{e}^{-ipx}\langle \frac{1}{2}\mathrm{Tr}[\gamma_5 D(x,x)]\Big(\frac{1}{2}\mathrm{Tr}[\gamma_5 D(0,0)] - \frac{Z}{2N_f}\nabla_\mu A^0_\mu(0)\Big)\rangle\,,\end{aligned} \tag{28}$$

since $\delta^x_A \hat{Q} = 0$. Taking, as before, the limit $p \to 0$ after $u \to 0$ in eq. (28), we get

$$\begin{aligned}\frac{F_\pi^2}{2N_f} m_{\eta'}^2\Big|_{u=0} &= \lim_{p\to 0}\lim_{u\to 0}\Big[(1-Z)\int d^4x\, \mathrm{e}^{-ipx}\langle \frac{1}{2}\mathrm{Tr}[\gamma_5 D(x,x)]\frac{1}{2}\mathrm{Tr}[\gamma_5 D(0,0)]\rangle + \\ &- \frac{Z}{1-Z}\frac{F_\pi^2}{2N_f} m_{\eta'}^2\Big]\,,\end{aligned} \tag{29}$$

where eq. (27) has been used in the l.h.s. and the last term comes from the contribution of the η' pole to the second term in the r.h.s. of eq. (28). Recalling that Z vanishes when $u \to 0$, we obtain

$$\frac{F_\pi^2}{2N_f} m_{\eta'}^2\Big|_{u=0} = \lim_{p\to 0}\lim_{u\to 0}\int d^4x\, \mathrm{e}^{-ipx}\langle \frac{1}{2}\mathrm{Tr}[\gamma_5 D(x,x)]\frac{1}{2}\mathrm{Tr}[\gamma_5 D(0,0)]\rangle\,. \tag{30}$$

Under the smooth-quenching hypothesis the limits $u \to 0$ and $p \to 0$ in this expression can be readily performed in the order indicated, as the first one simply amounts to setting the fermion determinant equal to unity. One gets in this way

$$\frac{F_\pi^2}{2N_f} m_{\eta'}^2 \Big|_{u=0} = \int d^4x \, \langle \frac{1}{2}\mathrm{Tr}[\gamma_5 D(x,x)] \frac{1}{2}\mathrm{Tr}[\gamma_5 D(0,0)] \rangle \Big|_{\mathrm{YM}} . \qquad (31)$$

The restriction to the pure YM theory, indicated in eq. (31), is an obvious consequence of the fact that, for a Green function with the insertion of only gluonic operators, neglecting the fermion determinant is tantamount to limiting the functional integral to the pure gauge sector of the theory.

A relevant question at this point is to ask for which value of N_c eq. (31) is supposed to be valid. The answer depends on the detailed behaviour of QCD with N_f. Various possibilities are logically envisageable.

1) In the most favorable situation, in which the limit $u \to 0$ of $\chi_{tL}(p)$ exists and is equal to the value it takes at $N_f = 0$ (fermion determinant equal to 1), the formula (31) is valid for any value of N_c and for each N_c it yields the mass of the η' meson to leading order in u in the world with the corresponding number of colours, without any $\mathrm{O}(1/N_c)$ corrections [17].

2) If quenching can be attained only in the limit in which the number of colours goes to infinity, then eq. (31) will yield a formula for the $m_{\eta'}^2$ valid up to $\mathrm{O}(1/N_c)$ corrections [15].

3) Finally it may happen that taking $u \to 0$ does not correspond to quenching. In this case one cannot pass from the fairly complicated eq. (30) to the more useful formula (31).

Equation (31) has precisely the same structure as the naive formula (5), when the expression (6) of the YM topological susceptibility is inserted in it. Remembering the meaning of $\frac{1}{2}\int d^4x \mathrm{Tr}[\gamma_5 D(x,x)]$ (eq. (18)), eq. (31) can be rewritten in the suggestive form

$$\frac{F_\pi^2}{2N_f} m_{\eta'}^2 \Big|_{u=0} = \lim_{V\to\infty} \frac{\langle (n_R - n_L)^2 \rangle}{V} , \qquad (32)$$

where $\langle (n_R - n_L)^2 \rangle$ is the expectation value of the square of the index of the GW fermion operator, D, and V is the physical volume of the lattice.

It may be interesting to see what are the implications of the hypothetical situation in which the η' mass would not vanish (linearly) with u. In this case the two limits $u \to 0$ and $p \to 0$ of χ_{tL} would commute, leading to the chain of relations

$$0 = \lim_{u\to 0}\lim_{p\to 0}\chi_{tL}(p) = \lim_{p\to 0}\lim_{u\to 0}\chi_{tL}(p) = \lim_{V\to\infty}\frac{\langle(n_R - n_L)^2\rangle}{V} \geq 0\,, \tag{33}$$

which imply either that the non-negative quantity $(n_R - n_L)^2$ vanishes identically for any gauge configuration or, at least, that the quantity $\langle(n_R-n_L)^2\rangle$ grows less than linearly with the number of lattice points.

4 Numerical results

In the form (32) the η' mass formula can be directly compared with overlap fermion simulation data, because the problem is reduced to counting the number of zero modes of the overlap-Dirac operator and measuring their chirality. There exist data both in 2 (abelian Schwinger model [45]) and in 4 ($SU(3)$ gauge theory [46]) dimensions.

4.1 2 dimensions: abelian Schwinger model

The validity of the WV formula can be explicitly checked in the case of the two-dimensional abelian Schwinger model [47], since the model is exactly soluble [47, 48]. Numerical checks are also possible, as there exist very recent simulations that make use of the overlap fermion formalism [45].

For the quantities of interest, one finds the formulae [49]

$$\hat{Q}(x) = \frac{e}{4\pi}\epsilon_{\mu\nu}F_{\mu\nu} \tag{34}$$

$$\chi_t(p) = \frac{e^2}{4\pi^2}\Big(1 - \frac{e^2/\pi}{p^2 + e^2/\pi}\Big)\,. \tag{35}$$

These formulae are for $N_f = 1$. The generalization to the case with N_f species of fermions can be found at the end of the Appendix.

By inspection one immediately recognizes that $\chi_t(p = 0) = 0$ and that there exists one single particle in the spectrum, a boson (the analogue of the η' in QCD) with mass

$$m^2_{\eta'} = \frac{e^2}{\pi}\,. \tag{36}$$

The residue of the η' pole is given by [49]

$$R_{\eta'}^2 = \left|\langle 0|\hat{Q}|\eta'\rangle\right|^2 = \Big(\frac{e^2}{\pi\sqrt{4\pi}}\Big)^2 . \tag{37}$$

As the negative term in eq. (35) is fully contributed by the fermion determinant, the η' mass formula in 2 dimensions reads

$$\frac{R_{\eta'}^2}{m_{\eta'}^2} = \chi_t(0)\Big|_{\text{quenched}} = \frac{e^2}{4\pi^2} . \tag{38}$$

Comparing eq. (38) with (37), one immediately checks the consistency of (38) with (36). Incidentally, looking back at eq. (31), we conclude that $F_{\eta'} = 1/\sqrt{2\pi}$.

Numerically one finds $\langle(n_R - n_L)^2\rangle = 2.7 \pm 0.4$, at $1/e^2 = 6$ in a lattice with $N = 24^2$ points [45], implying

$$\frac{\langle(n_R - n_L)^2\rangle}{N} = \frac{2.7 \pm 0.4}{24^2} = (4.7 \pm 0.7) \times 10^{-3} . \tag{39}$$

Although this number compares fairly well with the expected result (eq. (38))

$$\frac{e^2}{4\pi^2} = \frac{1/6}{4\pi^2} = 4.2 \times 10^{-3} , \tag{40}$$

further simulations at different β's and larger volumes are needed to have properly under control all sources of systematic errors.

4.2 4 dimensions: $SU(3)$ gauge theory

Using the spectral flow method [50], the expectation value of $(n_R - n_L)^2$ in an $SU(3)$ gauge theory has been computed for three lattice volumes ($N = 8^3 \times 12$, $8^3 \times 16$, $16^3 \times 8$) at $\beta = 5.85$ in the first paper of ref. [46]. The data show a fairly good scaling with N. If the value of the string tension $\sigma = (440 \pm 38\,\mathrm{MeV})^2$ [25] is used together with $a\sqrt{\sigma} = 0.2874(7)$ [51] to fix the lattice spacing, one finds ($V = Na^4$)

$$A = \frac{\langle(n_R - n_L)^2\rangle}{V} = \Big(198 \pm 20\,\mathrm{MeV}\Big)^4 , \qquad \beta = 5.85 . \tag{41}$$

The same authors [46] have also produced data at larger values of β and volumes. At $\beta = 6.0$ and $N = 16^3 \times 32$, using $a\sqrt{\sigma} = 0.2189(9)$ [51], they get

$$A = \frac{\langle (n_R - n_L)^2 \rangle}{V} = \Big(194 \pm 20\,\mathrm{MeV}\Big)^4\,, \qquad \beta = 6.0\,. \tag{42}$$

Errors in eqs. (41) and (42) have been computed by combining in quadrature the uncertainties on $\langle (n_R - n_L)^2 \rangle$, σ and $a\sqrt{\sigma}$. It is remarkable that the central value of A is quite stable with β and very near to the number required to match the actual value of the η' meson mass [17]. Clearly more work is needed (larger β values and volumes) before these encouraging indications are fully confirmed and the magnitude of the error is properly assessed.

5 Conclusions

In this paper we have given a derivation of the WV formula for the η' mass in lattice QCD, by exploiting the flavour-singlet axial WTIs of the theory. If fermions obeying the GW relation (15) are used, there exists a natural definition of topological density (eq. (19)), for which the naive form of the WV formula holds without the need of introducing any subtraction.

The validity of a formula of the WV type for the η' mass, i.e. of a formula that is telling us that the $\mathrm{O}(\Lambda_{\mathrm{QCD}})$ contribution to $m_{\eta'}$ originates from the breaking of the $U_A(1)$ symmetry due to the gluon anomaly, is a key test of our understanding of strong interaction dynamics, as described by QCD. It is reassuring that such a formula holds even beyond the formal continuum-like derivations given in refs. [15, 17].

In the literature essentially two kinds of approaches have been proposed to deal with the problem of computing of the topological susceptibility on the lattice, which have led to numerical values for A as good as those obtained here. The first one is based on a direct field theoretical definition of A [22] that takes into account the need for the renormalization of Q_L and the subtraction of the operators F^2 and $1\!\!1$ in the short distance expansion of $Q_L Q_L$. The second one makes use of the notion of "cooling" [52] to carry out the necessary operations of renormalization and subtraction. Both methods are reliable to the extent that they are able to capture the topological properties of the gauge field configurations that determine the number of zero modes of the Dirac operator. Simulations based on the geometrical definition of ref. [31] have not yet led to comparably good results [21].

We conclude by noting that a completely analogous set of arguments, as those developed in this paper, could be carried out for the pseudo-scalar meson (sort of η/π particle) belonging to the lightest supermultiplet of the $\mathcal{N}=1$ Super-YM gauge theory, the only difference being that in this case one would be dealing with Weyl fermions in the adjoint representation of the gauge group. In order to assess the numerical importance of gluino loops for the restoration of supersymmetry, it would be interesting to compare the values of the masses of the other two partners of the lowest lying supermultiplet, as they are obtained in quenched simulations [53], with the number one would derive for the mass of the η/π particle following the present analysis.

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Appendix

We present here a simple (and to our knowledge novel) derivation of a number of relations between certain hadronic observables and various quantities related to (the continuum limit of) the "topological susceptibility correlator" $\chi_t(p)$ (see eq. (25)).

The dispersion relation for $\chi_t(p)$

As $\chi_t(p)$ is a quantity of mass dimension 4, it will satisfy a three-times-subtracted dispersion relation [10] that we write in the form

$$\chi_t(p) = \chi_t(0) + \chi_t'(0)p^2 + \frac{1}{2}\chi_t''(0)(p^2)^2 + (p^2)^3 I\,, \tag{43}$$

[10] The same results as those obtained below follow, also if one starts with a dispersive integral having a smaller number of subtractions.

where for a properly defined correlator we have (see eq. (26))

$$\chi_t(0) = 0\,. \tag{44}$$

In eq. (43) I represents the dispersive integral involving $\mathrm{Im}\chi_t(p)$. It is useful to express I by separating out the η' contribution from the rest. We thus put

$$I \equiv \frac{1}{(m_{\eta'}^2)^3}\frac{R_{\eta'}^2}{p^2+m_{\eta'}^2} + \tilde{I}\,, \tag{45}$$

where $-R_{\eta'}^2$ is the full physical residue of the η' pole, which, as explicitly indicated, is negative-definite in Euclidean metric. This is a consequence of the fact that, by analytical continuation from the Minkowski region [49], the whole dispersive integral is negative-definite. This circumstance solves the famous sign problem discussed in [15].

The key observation at this point is that for the η' contribution the limits $p \to 0$ and $u \to 0$ do not commute, since (if) $m_{\eta'}^2 = \mathrm{O}(u)$. We then proceed by computing the two sides of eq. (43) by taking $u \to 0$ before $p \to 0$.

In doing so, in the l.h.s. of eq. (43) we simply get the quantity $\chi_t(p)$ in the quenched theory, i.e.

$$\chi_t(p)|_{\mathrm{quenched}} = \lim_{u\to 0}\chi_t(p)\,. \tag{46}$$

This follows from the assumption that, since $p \neq 0$, taking the limit $u \to 0$ (before $p \to 0$) is equivalent to neglecting the contribution of the fermion determinant (smooth-quenching hypothesis). In the r.h.s. we expand at fixed p^2 the η' contribution in powers of $m_{\eta'}^2/p^2 = \mathrm{O}(u/p^2)$ and then we match the resulting p^2 power behaviour with the Taylor expansion of $\chi_t(p)|_{\mathrm{quenched}}$ around $p^2 = 0$. We get in this way the relations

$$\chi_t''(0)|_{\mathrm{quenched}} = \lim_{u\to 0}\left[\chi_t''(0) + 2\frac{R_{\eta'}^2}{m_{\eta'}^6}\right]\,, \tag{47}$$

$$\chi_t'(0)|_{\mathrm{quenched}} = \lim_{u\to 0}\left[\chi_t'(0) - \frac{R_{\eta'}^2}{m_{\eta'}^4}\right]\,, \tag{48}$$

$$\chi_t(0)|_{\mathrm{quenched}} = \lim_{u\to 0}\left[\chi_t(0) + \frac{R_{\eta'}^2}{m_{\eta'}^2}\right]\,. \tag{49}$$

Since $\tilde{I}$ is a smooth function of u and p, which vanishes as $p \to 0$ with its first two derivatives, it does not give any contribution to the above equations.

The smooth-quenching hypothesis implies that the combinations appearing in the r.h.s. of eqs. (47) to (49) have a finite limit when $u \to 0$. As a consequence, they can be rewritten in the more expressive form

$$\frac{R^2_{\eta'}}{m^2_{\eta'}} = \chi_t(0)|_{\mathrm{quenched}} - \chi_t(0) + \mathrm{O}(u)\,, \tag{50}$$

$$-\frac{R^2_{\eta'}}{m^4_{\eta'}} = \chi'_t(0)|_{\mathrm{quenched}} - \chi'_t(0) + \mathrm{O}(u)\,, \tag{51}$$

$$2\frac{R^2_{\eta'}}{m^6_{\eta'}} = \chi''_t(0)|_{\mathrm{quenched}} - \chi''_t(0) + \mathrm{O}(u)\,. \tag{52}$$

In this way it clearly appears that, to leading order in u, the physical quantities in the l.h.s. of these equations are not affected by the presence of any possible counter-term, introduced to make the topological susceptibility correlator finite at $p \neq 0$ (see the discussion after eq. (10)). This immediately follows from the observation that the u-independent part of such counter-term, even if non zero, will cancel between quenched and unquenched quantities in the r.h.s. of eqs. (50), (51) and (52).

The η' mass formula

Owing to eq. (44), eq. (50), taken in the limit $u \to 0$, is nothing but the WV relation. To see this we recall that the residue of the η' pole is given by the formula

$$R^2_{\eta'} = \left|\langle 0|\hat{Q}|\eta'\rangle\right|^2. \tag{53}$$

To get an explicit expression of $R^2_{\eta'}$, it is sufficient to write the matrix element of $\hat{Q}$ appearing in eq. (53) in terms of the corresponding matrix element of the divergence of the flavour-singlet axial current, using the anomalous PCAC relation. As we are in the chiral limit, we get

$$2N_f\langle 0|\hat{Q}|\eta'\rangle = \langle 0|\nabla^\mu \hat{A}^0_\mu|\eta'\rangle\,. \tag{54}$$

We can express the r.h.s. of eq. (54) in terms of F_π, since, for the sake of deriving the WV formula, we are actually only interested in computing $R^2_{\eta'}$

in the limit $u \to 0$, where the pseudo-scalar meson decay constants, F_π and $F_{\eta'}$, coincide. Combining the equation [11]

$$\langle 0|\nabla^\mu \hat{A}^0_\mu|\eta'\rangle = \sqrt{2N_f}F_{\eta'}m^2_{\eta'}\,, \tag{55}$$

which defines $F_{\eta'}$, with (54), we obtain

$$\frac{R^2_{\eta'}}{m^2_{\eta'}}\Big|_{u=0} = \frac{F^2_{\eta'}m^2_{\eta'}}{2N_f}\Big|_{u=0} = \frac{F^2_{\pi}m^2_{\eta'}}{2N_f}\Big|_{u=0}\,. \tag{56}$$

Recalling that $F_\pi = \mathrm{O}(\sqrt{N_c})$ [16, 18] to leading order in u, we see that we consistently have $R^2_{\eta'}/m^2_{\eta'}|_{u=0} = \mathrm{O}(1)$. If we now put together eqs. (50) and (56), we finally get

$$m^2_{\eta'} = \frac{2N_f}{F^2_\pi}\chi_t(0)|_{\mathrm{quenched}} + \mathrm{O}(u^2)\,. \tag{57}$$

It is amusing to notice that eliminating $R^2_{\eta'}/m^2_{\eta'}$ between eqs. (51) and (52) provides a new formula for the η' mass, namely

$$m^2_{\eta'} = -2\,\frac{\chi'_t(0)|_{\mathrm{quenched}} - \chi'_t(0)}{\chi''_t(0)|_{\mathrm{quenched}} - \chi''_t(0)} + \mathrm{O}(u^3)\,, \tag{58}$$

which, as indicated above, is more accurate than the WV formula (57). It should be stressed that from eq. (58) $m^2_{\eta'}$ is expressed, up to $\mathrm{O}(u^3)$, in terms of differences between “quenched” and “full” quantities that are not affected by the presence of possible counter-terms in the definition of the topological susceptibility correlator at $p \neq 0$.

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[11] The numerical factor $\sqrt{2N_f}$ in equation (55) needs some explanation. The factor $\sqrt{2}$ comes from the fact that F_π is defined through the equation $\langle 0|\nabla^\mu A^{\pi^0}_\mu|\pi^0\rangle = F_\pi m^2_\pi$, where $\pi^0 = 2^{-1/2}(\bar{u}u - \bar{d}d)$, $A^{\pi^0}_\mu = \bar{q}\gamma_\mu\gamma_5\lambda^{\pi^0}q$ and $\lambda^{\pi^0} = \lambda_3/2$, with λ_3 the usual Gell-Mann matrix. The factor $\sqrt{N_f}$ is due to the fact that the flavour-singlet axial current, A^0_μ, is a sum over all light flavours with weight 1, while the wave function of the flavour-singlet meson has a $1/\sqrt{N_f}$ factor when expressed in terms of $\bar{q}q$ states. With these definitions F_π is of O(1) in N_f to leading order in N_c.

A formula for $\chi_t'(0)$

An interesting formula for $\chi_t'(0)$ can be derived from eq. (51). In fact, recalling eq. (52), the former can be identically rewritten in the more expressive fashion

$$\chi_t'(0) = \frac{F_\pi^2}{2N_f} + \left[\frac{R_{\eta'}^2}{m_{\eta'}^4} - \frac{F_\pi^2}{2N_f} + \chi_t'(0)|_{\text{quenched}}\right] + \mathrm{O}(u)\,, \tag{59}$$

where the first term is $\mathrm{O}(1/u)$ and the term in square brackets is of $\mathrm{O}(1)$, as follows from eq. (56). An expansion of this kind for $\chi_t'(0)$ can be useful in connection with the discussion of the proton spin crisis problem, given in ref. [37], where it was noticed that, in the limit in which $\chi_t'(0)$ is identified with $F_\pi^2/2N_f$, one recovers the Ellis–Jaffe sum rule [54]. It would be interesting to see whether the correction in square brackets goes in the right direction for solving the proton spin puzzle.

For the study of the proton spin problem one is directly interested in $\chi_t'(0)$ itself and not in "quenched"–"full" differences, like the combinations (50), (51) and (52) appearing in the formulae (57) and (58) for the η' mass. Thus the question arises whether the quantity $\chi_t'(0)$ can be defined in a way amenable to unambiguous numerical simulations. This is the case only if terms proportional to p^2 are absent in the polynomial expansion of the counter-term, $\mathrm{CT}(p)$. However, in a (lattice) regularized theory the presence of a quadratically divergent term of the type $p^2 1\!\!1/a^2$ cannot be excluded and will thus have to be compensated for. This means that there is no obvious way to define $\chi_t'(0)$ in a way suitable for numerical simulations, at least from these simple considerations only.

The two-dimensional case

We conclude by noticing that in the two-dimensional abelian ($N_c = 1$) Schwinger model with N_f species of fermions, one can directly verify the validity of eqs. (50) to (52), which, in fact, hold exactly without $\mathrm{O}(u = N_f)$ corrections. It is sufficient to observe that the generalization of eq. (35) to arbitrary N_f reads

$$\chi_t(p) = \frac{e^2}{4\pi^2}\left(1 - \frac{N_f e^2/\pi}{p^2 + N_f e^2/\pi}\right)\,, \tag{60}$$

while the ratio (38) is independent of N_f.

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