TOPOLOGICAL SUSCEPTIBILITY IN LATTICE QCD
AND PERTURBATION THEORY

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Abstract

We consider the definition of topological susceptibility suggested by the anomalous $U_A(1)$ Ward Identity in lattice QCD with Wilson's fermions and show that, in the limit of zero renormalized quark mass, its perturbative expansion is zero to all orders. This definition is thus suitable for Monte Carlo simulations.

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A distinctive feature of any theory of strong interactions, such as QCD, should be its capability of explaining the spectrum of low lying pseudoscalar mesons as a result of the spontaneous breaking of the chiral $SU(N_f) \times SU(N_f)$ flavour symmetry down to vector $SU(N_f)$.

Although one can imagine a consistent picture in which such dynamical breaking occurs, one has, in QCD, the problem of explaining why there is no Goldstone boson associated to the flavourless axial $U_A(1)$ symmetry that the theory possesses at the classical level. A solution to this problem can be envisaged^{(1),(2)} starting from the observation that the corresponding flavourless $U_A(1)$ current is anomalous:⁽³⁾

$$\partial_\mu J_\mu^5(x) = 2 N_f Q(x) + D(x) \quad (1)$$

where

$$J_\mu^5(x) = \sum_{i=1}^{N_f} \bar{\Psi}_i(x) \gamma_\mu \gamma_5 \Psi_i(x) \quad (2)$$

$$D(x) = 2i \sum_{i=1}^{N_f} m_i \bar{\Psi}_i(x) \gamma_5 \Psi_i(x)$$

and

$$Q(x) = \frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_{\mu\nu}^a(x), \quad \tilde{F}_{\mu\nu}^a = \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} F_{\rho\sigma}^a \quad (3)$$

is, in Euclidean region, the topological charge density. g and m_i are the gauge coupling constant and the quark masses.

A formula for the singlet pseudoscalar meson can be obtained either by requiring, as in ref.(4), the cancellation of the Θ -dependence of the vacuum energy of the pure gauge part of the theory against the contribution coming from massless quark loops, or by asking, as in ref.(5), that anomalous and non-anomalous Ward identities are saturated order by order in the number of quark loops. In both cases in the chiral limit ($m_i \rightarrow 0$) one gets:

$$m_{\text{singlet}}^2 = \frac{2 N_f}{F_\pi^2} A \quad (4)$$

where

$$A = \int d^4x \langle Q(x) Q(0) \rangle \Big|_{\text{no quark loops}} \quad (5)$$

is a quantity which only depends on the gauge part of the theory and F_π is the pion decay constant ($F_\pi \simeq 95$ MeV). Phenomenologically one finds^(*) $A \simeq (180 \pm 50 \text{ MeV})^4$

To check the validity of eq.(4), Montecarlo methods have been employed, using different definitions (see refs. (7), (8) and (9)) of the topological charge density.

The first attempts⁽⁷⁾ to measure A used a lattice definition of Q with no topological meaning and gave a much too small value as compared to the phenomenological one both in the $SU(2)_c$ and $SU(3)_c$ cases. The trouble with these definitions is that the lattice version of A has a non zero perturbative expansion in $1/\beta = g^2/2N_c$ which is numerically competing with the non perturbative (exponentially small) renormalization group invariant behaviour $(e^{-\beta/4N_c\beta_1})^4$ where $\beta_1 = \frac{11}{3} \frac{N_c}{16\pi^2}$ is the first coefficient of the β -function and the exponent 4 is the mass dimension of A . The existence a perturbative tail, besides rendering numerically delicate the identification of the physically interesting non-perturbative behaviour of A , raises the conceptual point of the meaning of subtracting a (divergent) perturbative term in order to get non perturbative information.⁽¹⁰⁾

In refs.(8) and (9) two different definitions of Q are considered in the $SU(2)_c$ case, that are related to the gene-

(*) A more accurate estimate⁽⁶⁾ taking into account $SU(3)_f$ breaking effects gives a significantly lower value for A , namely $(110 \pm 50 \text{ MeV})^4$. We wish to thank S.Narison for a discussion on this point.

ral expression for the topological charge, q , defined by Luscher⁽¹¹⁾ (see also ref.(12)). In the construction of ref.(11) a smoothing procedure is defined locally on each hypercube that allows one to associate to each (non-exceptional) lattice configuration on a four-dimensional torus an $SU(2)$ principal bundle. q is then identified with the topological charge of the bundle. Owing to its topological meaning q is free from perturbative tail and it is automatically integer-valued. The definitions given in refs.(8) and (9) differ from the one proposed by Luscher and between them because of the different smoothing procedure employed.

In this paper we want to discuss the definition of $Q(x)$ which is directly suggested by the lattice analog of eq.(1)⁽¹³⁾⁻⁽¹⁶⁾ in a theory with Wilson fermions. This definition has the advantage of having a formal expression which is independent of the gauge group and it does not necessitate any smoothing procedure.

As is well known in continuum QCD⁽¹⁷⁾ and, as will be obvious in the present lattice version, the two operators on the r.h.s. of eq.(1) are mixed by the renormalization procedure needed to define two separately finite operators. We shall show that, if a properly defined chiral limit is taken, it is possible to get a well-defined expression for $Q(x)$. Besides, the expression for A will be free from perturbation theory.

We start by writing the action of lattice QCD. To avoid fermion doubling we follow Wilson⁽¹⁸⁾ and include in the action a term which breaks explicitly the chiral invariance. In the euclidean region, introducing the dependence upon the θ -angle, as discussed in refs.(15) and (16), we have in the case of only one flavour:

$$\begin{aligned}
 S &= S_g(\beta, U) + S_f(U, \theta; M) \equiv \\
 &\equiv -\frac{\beta}{2N_c} \sum_P U_P - a^4 \sum_{m,l} \bar{\psi}_m (\not{D} - e^{i\theta \gamma_5} W + M)_{ml} \psi_l
 \end{aligned} \tag{6}$$

where a is the lattice spacing, M is related to the bare quark mass and

$$U_P = \text{Tr} [U_\mu(n) U_\nu(n+\mu) U_\mu^\dagger(n+\nu) U_\nu^\dagger(n)] \quad (7a)$$

$$(D_\mu)_{ml} = \frac{1}{2a} [U_\mu(n) \delta_{l, n+\mu} - U_\mu^\dagger(l) \delta_{n, l+\mu}] \quad (7b)$$

$$(W)_{ml} = \frac{\pi}{2a} \sum_{\mu=1}^4 [U_\mu(n) \delta_{l, n+\mu} + U_\mu^\dagger(l) \delta_{n, l+\mu} - 2\delta_{n,l}] \quad (7c)$$

As usual $U_\mu(n)$ denotes the gauge group element associated with the link $(n, n+\mu)$.

Performing the fermion integration, we can define a fermion partition function Z_f in the external field U :

$$Z_f(U, \theta; M) \equiv \text{Det} (\not{D} - e^{i\theta\gamma_5} \not{W} + M), \quad (8)$$

where the determinant is over space-time, spin and colour indices. The partition function of the complete theory can be written in terms of Z_f as follows:

$$Z(\beta, \theta; M) = \int (dU) e^{-S_g(\beta, U)} Z_f(U, \theta; M). \quad (9)$$

Two comments are in order:

- i) as usual, to trace the effect of the Wilson term, a factor r has been introduced in front of $\not{W}$. No physical quantity should depend on it.
- ii) In the case of many flavours one can define vector and axial currents which have, at least in the naive $a \rightarrow 0$ limit, the correct Bardeen⁽¹⁹⁾ flavor anomalies⁽²⁰⁾. They originate from the Wilson term, but in the naive continuum limit they are r -independent⁽²⁰⁾.

The crucial point is that, although under the transformation

$$\begin{aligned} \psi_n &\rightarrow e^{\frac{i\theta}{2}\gamma_5} \psi_n \\ \bar{\psi}_n &\rightarrow \bar{\psi}_n e^{\frac{i\theta}{2}\gamma_5} \end{aligned} \quad (10)$$

S_f is formally θ independent in the limit $M \rightarrow 0$ (this is the lattice counterpart of the statement that Z in the continuum is θ independent in presence of massless quarks), in lattice QCD this is not a well defined statement until we specify what we mean by $M \rightarrow 0$. As already noticed in fact, W explicitly breaks chirality so that, even starting with vanishing quark masses, we will have to cope with radiative corrections which will drive masses away from zero. It is thus clear that, if we want to repeat the Witten-Veneziano argument for the η' mass, we have to keep the renormalized quark mass at zero. To see how this can be done, we rewrite S_f in the form:

$$S_f(0, \theta'; m', m) = \sum_{n, \ell} \bar{\psi}_m \left[\not{D} - e^{i\theta'} \gamma_5 (\not{W} - m') + m \right]_{n, \ell} \psi_\ell \quad (11)$$

where we have redefined the mass and the angle through the equations:

$$\begin{aligned} m \cos \theta' &= M \cos \theta - m \\ m \sin \theta' &= M \sin \theta \end{aligned} \quad (12)$$

m' is then fixed in such a way that the renormalized quark mass, defined as the position of the pole of the quark propagator, is located at zero order by order in perturbation theory when $m \rightarrow 0$. This means that, writing the inverse quark propagator for small momenta as $\not{D} + \Sigma(p, g^2, r, m, m')$ we fix m' by the condition:

$$\lim_{m \rightarrow 0} \Sigma(0, g^2, r, m', m) = 0 \quad (13)$$

We shall indicate by $m'_{cr} = m'_{cr}(r, g^2)$ the solution of eq. (13) and we put

$$\not{W}_{cr} \equiv \not{W} - m'_{cr} \quad (14)$$

We will also denote by $\hat{Z}(\beta, \theta; m)$ the partition function of the theory with fermion action (11) with m' equal to m'_{cr} and we define:

$$Z^{cr}(\beta) = \lim_{m \rightarrow 0} \hat{Z}(\beta, \theta; m). \quad (15)$$

$Z^{cr}(\beta)$ describes the theory in the chiral limit, while m in $\hat{Z}(\beta, \theta; m)$ plays the role of an infra-red cut-off. We notice that the redefinition (12) tells us what is to be called the θ angle of the theory. The chiral limit as defined by eq.(13) gives a definition of θ which parallels the continuum one, in the sense of the θ -independence of Z^{cr} .

We now have two alternative ways to compute the η' mass.

The first one is to derive the lattice analogue of eq.(1) in order to identify what should be called Q_L , i.e. the "lattice topological charge density". From it, through (5) we can get the expression of A to be inserted in eq.(4).

The second way is to use the θ -independence of the vacuum energy to identify the lattice analog of the pure Yang Mills quantity to be used in eq.(4).

Let us start with the first method namely let us perform the local change of variables⁽¹⁵⁾

$$\psi_m \rightarrow e^{i\alpha_m \gamma_5} \psi_m \quad (16)$$

$$\bar{\psi}_m \rightarrow \bar{\psi}_m e^{i\alpha_m \gamma_5} \quad (17)$$

The invariance condition $\partial Z^{cr} / \partial \alpha_m |_{\alpha_m=0} = 0$ gives us the following Ward identity:

$$\partial_\mu J_\mu^5(m) = \chi(m) + 2m j^5(m) \quad (18)$$

where

$$J_\mu^S(m) = \frac{i}{2} [\bar{\Psi}_m \gamma_\mu \gamma_5 U_\mu(m) \psi_{m+\mu} + \bar{\Psi}_{m+\mu} \gamma_\mu \gamma_5 U_\mu^\dagger(m) \psi_m], \quad (19)$$

$$j^S(m) = i \bar{\Psi}_m \gamma_5 \psi_m, \quad (20)$$

$$\begin{aligned} \chi(m) = & -\frac{i\tau}{2a} \sum_{\mu=1}^4 [\bar{\Psi}_m \gamma_5 U_\mu(m) \psi_{m+\mu} + \bar{\Psi}_{m+\mu} \gamma_5 U_\mu^\dagger(m) \psi_m + \\ & + \bar{\Psi}_{m-\mu} \gamma_5 U_\mu(m-\mu) \psi_m + \bar{\Psi}_m \gamma_5 U_\mu^\dagger(m-\mu) \psi_{m-\mu} + \\ & - 4 \left(1 - \frac{am'_c}{4\tau}\right) \bar{\Psi}_m \gamma_5 \psi_m \end{aligned} \quad (21)$$

and

$$(\partial_\mu f)(m) = \frac{1}{a} [f(m) - f(m-\mu)]. \quad (22)$$

Taking into account the previous discussion on the definition of W_{cr} , the structure of eq.(18) suggests the identification:

$$Q_L(m) = \chi(m) \quad (23)$$

A more useful version of the Ward identity (18) is obtained by summing over all space-time points and integrating over fermions. In this way one gets:

$$\text{Tr}(\gamma_5 W_{cr} G_{cr}) = m \text{Tr}(\gamma_5 G_{cr}) \quad (24)$$

where

$$G_{cr} = (\not{D} - W_{cr} + m)^{-1} \quad (25)$$

is the lattice fermion propagator.

The identification (23) is confirmed by the results of ref.(15) where it is proved that for sufficiently smooth

field configurations:

$$\lim_{a \rightarrow 0} \text{Tr} [\gamma_5 W (\not{D} - W + M)^{-1}] = \frac{g^2}{32\pi^2} \int d^4x F_{\mu\nu}^a \tilde{F}_{\mu\nu}^a, \quad (26)$$

independently of M . Of course while establishing eq.(25) the "naive" continuum limit has been considered, that is M and W are the bare quantities defined by eqs.(6) and (7). Recalling eqs.(23)-(25) and all our previous discussion about the chiral limit, we put:

$$A(\beta) = \lim_{m \rightarrow 0} A(\beta, m) \quad (27a)$$

$$A(\beta, m) = \frac{m^2}{Z_g V T} \int (d\nu) e^{-S_g(\beta, \nu)} [\text{Tr}(\gamma_5 G_\nu)]^2 \quad (27b)$$

where

$$Z_g = \int (d\nu) e^{-S_g(\beta, \nu)}. \quad (28)$$

The fundamental observation here is that, as shown in detail in ref.(21), the perturbative expansion of $A(\beta)$ is identically zero. This is due to the infra-red finiteness at $m \rightarrow 0$ of the quantity multiplied by m^2 in eq.(27b). Of course if m is different from zero, a perturbative tail is present which, for small m behaves as m^2 . This has been verified by a direct calculation up to order $1/\beta^3$ in ref.(21).

The definition (27) together with eq.(14) was essentially the one adopted in ref.(22) to get an estimate of the η' mass. In that paper, however, no attention was paid to the problem of the possible existence of a perturbative tail.

We also observe that in a "hopping parameter" expansion of $A(\beta, m)$ one gets to lowest order the kind of expressions used in ref.(7).

The alternative method to define A is to repeat the Witten-Veneziano argument directly on the lattice starting from:

$$\lim_{m \rightarrow 0} \frac{\partial^2}{\partial \theta^2} \frac{1}{VT} \log \hat{Z}(\beta, \theta; m) \Big|_{\theta=0} = 0 \quad (29)$$

After performing the fermion integration we get:

$$\begin{aligned} & \lim_{m \rightarrow 0} \hat{Z}^{-1}(\beta, \theta=0; m) \int (d\psi) e^{-S_g(\beta, \psi)} \text{Det}(\not{D} - \not{W}_{cr} + m) \cdot \\ & \cdot \frac{1}{VT} \left[(m \text{Tr}(\not{D}_S G_{cr}))^2 - \text{Tr}(m G_{cr} + m^2 \not{D}_S G_{cr} \not{D}_S G_{cr}) \right] = 0 \end{aligned} \quad (30)$$

To identify the analog of the quantity (5) to be inserted into eq.(4), it is enough to split the determinant as:

$$\text{Det}(\not{D} - \not{W}_{cr} + m) = 1 + [\exp \text{Tr} \log(\not{D} - \not{W}_{cr} + m) - 1] \quad (31)$$

and rewrite eq.(30) in the form:

$$\begin{aligned} & \lim_{m \rightarrow 0} \frac{1}{Z_g} \int (d\psi) e^{-S_g(\beta, \psi)} \cdot \\ & \cdot \frac{1}{VT} \left[(m \text{Tr}(\not{D}_S G_{cr}))^2 - \text{Tr}(m G_{cr} + m^2 \not{D}_S G_{cr} \not{D}_S G_{cr}) \right] = \\ & = \lim_{m \rightarrow 0} \frac{1}{Z_g} \int (d\psi) e^{-S_g(\beta, \psi)} [\exp \text{Tr} \log(\not{D} - \not{W}_{cr} + m) - 1] \cdot \\ & \cdot \frac{1}{VT} \left[(m \text{Tr}(\not{D}_S G_{cr}))^2 - \text{Tr}(m G_{cr} + m^2 \not{D}_S G_{cr} \not{D}_S G_{cr}) \right]. \end{aligned} \quad (32)$$

The quantity in the l.h.s. of (32) should now be identified with A. This expression does not coincide with the one found

in the previous way (see eqs.(27) and (28)). However one should note that:

- i) the naive $a \rightarrow 0$ limit of the second term in the l.h.s. of eq.(32) is zero⁽¹⁶⁾,
- ii) if one has N_f flavours and considers the analog of eq. (29) in this case, i.e. one takes the second derivative of $Z(\beta, \varphi_1, \dots, \varphi_{N_f}; m)$ with respect to two different chiral angles φ_i and φ_j ($\sum_i \varphi_i = \theta$), one would not get the additional term $\text{Tr}(m G_{\text{cr}} + m^2 \gamma_5 G_{\text{cr}} \gamma_5 G_{\text{cr}})$ in eq.(32),
- iii) at least in the continuum this extra term has a different N_c behaviour from the others in eq.(32) so it should be zero (and it actually is) by itself. In any case, on the lattice also, the perturbative tail of this additional term is absent in the chiral limit.

We have thus shown that A , as defined through eqs.(27) is identically zero in perturbation theory in the chiral limit. This of course does not mean that A is identically zero. In fact we expect $\text{Tr}(\gamma_5 G_{\text{cr}})^2$ to diverge as m^{-2} as $m \rightarrow 0$ for configurations such that $\text{Det}(\not{D} - W_{\text{cr}})$ vanishes. Precisely these (non-perturbative) configurations will contribute to a non-zero η' mass.

To conclude we want to make a comment on the feasibility of a Monte Carlo simulation of the formulae (27). The inversion of the matrix $(\not{D} - W_{\text{cr}} + m)_{nm}$ requires apparently an amount of time growing like L^2 , L being the number of space-time points of the lattice. However, being only interested in the trace of G_{cr} , it should be possible to use the Langevin method⁽²³⁾ which allows the direct computation of the trace with computer time growing as L only.^(*) As for the values of m'_{cr} to be used in A , one should proceed as in the case of the evaluation of hadron masses and fix it by the requirement that the pion is massless.⁽²²⁾.

(*) We are indebted to G.Martinelli for a discussion on this point.

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