ON THE TOPOLOGICAL STRUCTURE OF THE VACUUM IN SU(2) AND SU(3) LATTICE GAUGE THEORIES

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We present Monte Carlo measurements of the net topological charge of the vacuum in SU(2) and SU(3) lattice gauge theories. In both cases there is no evidence of any topological structure, and the values obtained are a factor of O(100) smaller than expectations based on analyses of the U(1) problem. Moreover we find a strong sensitivity to the lattice size and to the boundary conditions imposed on the lattice. We comment on the physical significance of these results, establish criteria for the reliable performance of such calculations, and remark on the possibly detrimental impact of these findings on the calculation of hadron spectra.

The topological charge density, $F\tilde{F}(x)$, of SU($N \geqslant 2$) non-abelian gauge theories receives its name because in the semiclassical limit ($\hbar \to 0$) it measures the presence of instantons and anti-instantons [1] ‡1. Because of asymptotic freedom (and because the only place the coupling, g^2, appears is in the product $\hbar g^2$) one can argue that (anti)-instantons are the dominant non-perturbative field fluctuations in the region of sizes between the very small, where only perturbative fluctuations are to be found, and the moderately large, ~1 fm, where complex and not well-understood non-perturbative fluctuations must dominate. Instantons may thus affect the detailed structure of hadrons [3]. Moreover instantons may be part of the mechanism causing chiral symmetry breaking [3]: indeed there are some numerical indications that chiral symmetry breaking occurs on smaller size scales than hadron formation [4] (which would help to clarify the current and constituent roles that quark masses play ‡2 and the important non-perturbative fluctuations on these smaller size scales are, presumably, instantons.

The topological charge density has also had a crucial role to play in resolving the U(1) problem [6]. The qualitative resolution of this problem was originally given in terms of instantons [6]. More recently however more quantitative attacks on this problem have involved considerations [7] of the large N limit [8] of

‡1 For pedagogical reviews see ref. [2].

‡2 For a recent summary see ref. [5].

the gauge theory, and effective low-energy lagrangians [9] embodying this large N physics. These latter approaches require that the fluctuations of the integrated topological charge should have a certain size:

$$\left\langle \left(\frac{g^2}{16\pi^2 N} \int d^4x\, F\tilde{F}(x) \right)^2 \right\rangle \approx VT(180\ \mathrm{MeV})^4\,, \qquad (1)$$

where VT is the volume of space–time and $g/\sqrt{N}$ is the usual coupling in the SU(N) gauge theory. The normalisation is such that one instanton contributes

$$\frac{g^2}{16\pi^2 N} \int d^4x\, F\tilde{F}(x) = 1\,, \qquad (2)$$

so that (1) could be interpreted as saying that on average a volume of (euclidean) space–time of 1 fm^4 will contain roughly 1 net instanton or anti-instanton. There is however no obvious connection between the arguments leading to (1) and instantons: indeed the usual [7] (although only partially correct [‡3]) prejudice is that the $\exp(-8\pi^2 N/g^2)$ factor in the density of instantons (coming from their non-trivial classical action) will ensure that they do not contribute to any finite order in the $1/N$ expansion. One should therefore treat (1) and the instanton content of $F\tilde{F}$ as separate expectations; although we note that (1) is not an unreasonable value in the context of a typical [‡4] dilute gas of (anti-)instantons. Note finally that (1) is derived for full QCD with fermions; the expectation value is however to be evaluated in the *pure* gauge theory without quarks.

To test whether the theory does indeed give (1), Di Vecchia et al. [12] evaluated the left hand side of (1) for the SU(2) lattice regularised gauge theory [13], using the Monte Carlo technique [14] on a small 4^4 lattice with periodic boundary conditions. The result was ($\sim$50 MeV)^4 in place of the (180 MeV)^4 in (1) – a dramatic discrepancy by a factor of over 100.

In this paper we shall pursue this problem considerably further. As a by-product of our lattice Monte Carlo calculations of the glueball mass spectrum [15] and glueball internal structure [16] in SU(2) and SU(3) gauge theories, we have obtained measurements of two $F\tilde{F}$ operators (essentially those used in ref. [12]) for both SU(2) *and* SU(3). Moreover, in addition to extracting the value of the left hand side of (1) (as was done for SU(2) in ref. [12]), we also consider it interesting to investigate the distribution of values of $\int F\tilde{F}(x)\, d^4x$ to see if there is any sign of the lattice containing instantons. We shall in fact find both no evidence of instantons and a dramatic discrepancy with (1), for both SU(2) and SU(3). But there will be more to it than just that.

To begin with we summarize briefly what was done in ref. [12]. The authors used two lattice definitions of $F\tilde{F}(x)$:

$$F\tilde{F}_{\mathrm{A}}(n) = -\frac{1}{2^4 \cdot 32\pi^2} \sum_{(\mu,\nu,\rho,\sigma)=\pm 1}^{\pm 4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \times \mathrm{tr}(U_{n,\mu} U_{n+\mu,\nu} U_{n+\mu+\nu,\rho} U_{n+\mu+\nu+\rho,\sigma} \times U^+_{n+\nu+\rho+\sigma,\mu} U^+_{n+\rho+\sigma,\nu} U^+_{n+\sigma,\rho} U^+_{n,\sigma})\,, \qquad (3)$$

$$F\tilde{F}_{\mathrm{B}}(n) = -\frac{1}{2^4 \cdot 32\pi^2} \sum_{(\mu,\nu,\rho,\sigma)=\pm 1}^{\pm 4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \times \mathrm{tr}(U_{n,\mu\nu} U_{n,\rho\sigma})\,, \qquad (4)$$

where $\tilde{\epsilon}_{\mu\nu\rho\sigma}$ is an extension [12] of the usual $\epsilon_{\mu\nu\rho\sigma}$ tensor such that $\tilde{\epsilon}_{1\nu\rho\sigma} = -\tilde{\epsilon}_{-1\nu\rho\sigma}$ etc., the $U_{n,\mu}$ are link variables out of the site n in the μ direction (positive or negative), and $U_{n,\mu\nu}$ represents the plaquette in the $\mu\nu$ plane at site n. The calculations were performed in SU(2) on a 4^4 lattice for a range of couplings, $\beta(\equiv 4/g^2) \approx 0.5$ to 4.5. These operators receive perturbative lattice contributions and to obtain the desired non-perturbative piece of $\langle(\Sigma F\tilde{F})^2\rangle$, these must be subtracted. This was done by calculating the leading piece, and fitting the data for $\beta \geqslant 2.8$ to obtain the non-leading (but large) perturbative contributions. The resulting non-perturbative piece is found to have the desired renormalisation group behaviour for $2.2 \lesssim \beta \lesssim 2.4$; but is a factor of O(100) too small to fit (1).

In our SU(2) calculations we use $F\tilde{F}_{\mathrm{B}}$. In our SU(3) calculations we use $F\tilde{F}_{\mathrm{A}}$ but confined to the

[‡3] A careful calculation is needed because the number of ways of embedding an instanton gives a factor growing exponentially in N. It turns out that the pure dilute gas of (anti) instantons does indeed vanish as $N \to \infty$; however this behaviour is so marginal that the inclusion of first order interactions (à la ref. [3]) reverses this conclusion. It is therefore quite possible that instantons survive the $N \to \infty$ limit. For the calculation, see ref. [10].

[‡4] For the formulae for such estimates see for example ref. [11].

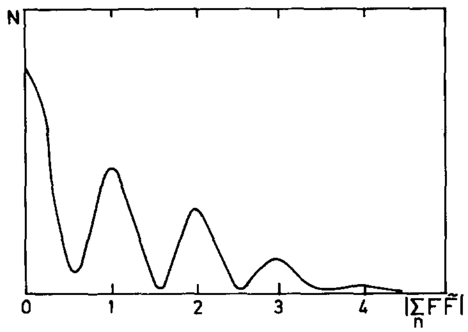

Fig. 1. A schematic view of the total topological charge on a lattice in the presence of instantons.

piece of the sum with $\mu = 4$. From now on we refer to these simply as $F\tilde{F}$.

Our calculations will be as follows. For SU(3) we have results on a $4^3 \cdot 8$ lattice at $\beta = 5.7$ [for SU(3), $\beta = 6/g^2$]. For SU(2) we have results for an 8^4 lattice at $\beta = 2.3$. In both cases we use the standard Wilson action [13] and periodic boundary conditions. We also have results on a 4^4 lattice with periodic boundary conditions at $\beta = 2.3$ and this enables us to cross-check with ref. [12]. At $\beta = 2.3$ the ratio of our value of $\langle (\Sigma F\tilde{F})^2 \rangle$ (based on 900 sweeps) to that of ref. [12] is 0.97 ± 0.085, which reassures us that we are doing the same kind of calculation.

In fig. 1 we show the kind of curve we might expect when we measure $\Sigma_n F\tilde{F}(n)$; the peaks about integers are the signatures of instantons on the lattice, and the fact that we have finite widths peaks rather than δ-functions is due to the perturbative contributions.

In fig. 2 we show the measured distribution for our SU(3) data on a $4^3 \cdot 8$ lattice at $\beta = 5.7$. We see no instantons.

In fig. 3 we show our SU(2) data taken on an 8^4 lattice at $\beta = 2.3$. Again no instantons.

We now worry whether using periodic boundary conditions biases us towards $\Sigma F\tilde{F} = 0$. The worry is based on the following argument [made for SU(2)]. The variables which are periodic are the link matrices, U_μ, which may be expressed as

$$U_\mu = \exp(\mathrm{i}a\bar{A}_\mu) , \tag{5}$$

where the matrix-valued field variable $\bar{A}_\mu$ can be written

$$\bar{A}_\mu = A_\mu^a \sigma^a = A_\mu \hat{c}^a \sigma^a , \tag{6}$$

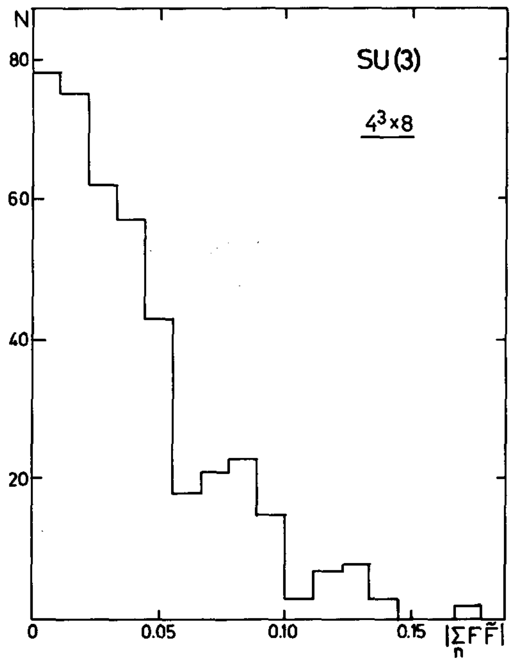

Fig. 2. The total SU(3) topological charge (modulus) on a $4^3 \cdot 8$ lattice with periodic boundary conditions at $\beta = 5.7$. (The horizontal scale is in units of winding number).

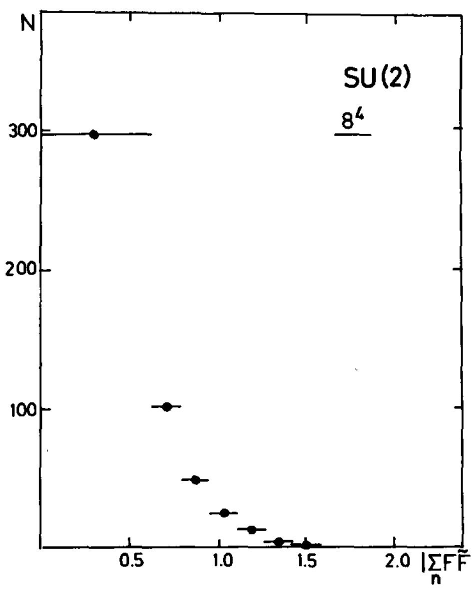

Fig. 3. The total SU(2) topological charge (modulus) on an 8^4 lattice with periodic boundary conditions at $\beta = 2.3$. The scale is as in fig. 2.

where $\hat{c}$ is the direction in SU(2) space of $\bar{A}_\mu$. Periodicity may be generically expressed as

$$U_\mu(R,\theta) = U_\mu(R,\theta+\pi)\,, \tag{7}$$

which becomes in terms of (5) and (6)

$$\bar{A}_\mu(R,\theta) = \bar{A}_\mu(R,\theta+\pi) + (2\pi m/a)\,\hat{c}^a\sigma^a \tag{8}$$

(where m and $\hat{c}$ can depend on μ). In the continuum limit, keeping R fixed at any desired value, continuity in the $\bar{A}$ will demand dropping the $1/a$ term in (8). Hence we obtain periodic boundary conditions in the gauge potential $\bar{A}_\mu$, and the net topological charge must vanish (because in the continuum it can be expressed as a surface integral). Of course the above is only one way to approach the continuum limit. Nonetheless to the extent that we are indeed close to the continuum limit we expect the periodic boundary conditions to bias us to $\Sigma F\tilde{F} \approx 0$ (in this context we find the comments in ref. [12] to be overoptimistic).

To eliminate the effects of boundary conditions we took a 4^4 sublattice of our 8^4 lattice and measured $\Sigma_n F\tilde{F}$ on this sublattice alone. This sublattice now is immersed within a "heat bath" provided by the larger lattice. Since the correlation length at $\beta = 2.3$ is about one lattice spacing, the 4^4 sublattice will have little dynamical contact with the boundaries of the 8^4 host lattice. Such an arrangement mimics closely the desired situation where we would make measurements on a piece of an infinite volume of space–time; and so provides the "best possible" boundary conditions [‡5]. The results for this 4^4 sublattice are plotted in fig. 4. There are no instantons to be seen.

Using the usual string tension values [15,17] the volume of our SU(3) $4^3 \cdot 8$ lattice is ~4 fm^4, of our SU(2) 8^4 lattice is ~11 fm^4, and of the SU(2) 4^4 sublattice is ~0.7 fm^4. So our lattices are certainly big enough to have instantons – which was obvious anyway since all (except the last) were used to calculate the glueball mass spectrum.

‡5 One might think of trying boundary conditions such as $\bar{A}_\mu(R,\theta) = -\bar{A}_\mu(R,\theta+\pi)$ under which surface integrals no longer vanish. We did. The effects of these boundary conditions on such quantities as the average action per plaquette are felt two or three sites inwards from the boundaries because, unlike periodic boundary conditions, they break translation invariance – the boundaries are a special place; so one must work on very large lattices with such boundary conditions.

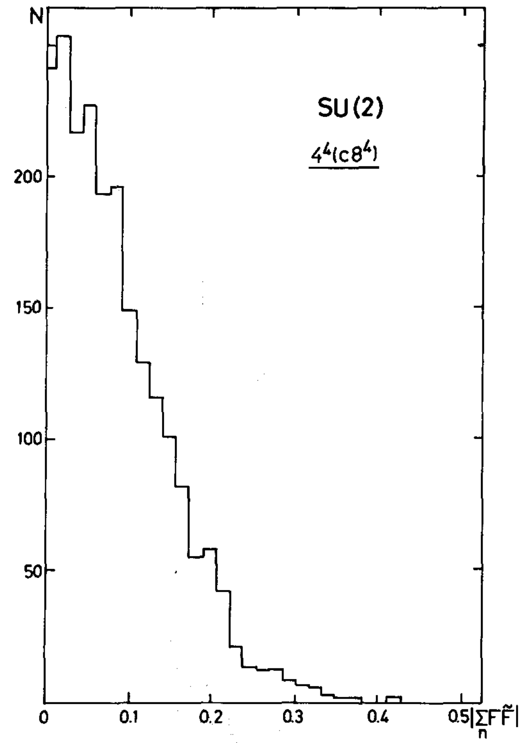

Fig. 4. The total SU(2) topological charge (modulus) on a 4^4 lattice embedded in a larger 8^4 lattice at $\beta = 2.3$. The scale is as in fig. 2.

Having found no evidence for instantons on our lattice, let us ask how our data compares with (1). As we remarked earlier (1) is equivalent to requiring about 1 net (anti) instanton per fm^4. If we examine figs. 2–4 normalised by the volumes of the previous paragraph we see that the discrepancy between our measured values of the left hand side of (1) and the right hand side is again O(100) – both for SU(2) and for SU(3).

We emphasize that this conclusion does *not* depend on the details of the perturbative subtraction: in this range of coupling, if the non-perturbative piece of $\langle(\Sigma F\tilde{F})^2\rangle$ were as large as suggested by (1) it would be a factor ~50 larger than the perturbatively calculated piece. The only reason it was necessary to be careful about the perturbative subtraction in ref. [12], was because in fact the non-perturbative piece is so much smaller than expected.

Unlike our earlier qualitative search for instanton effects, the testing of (1) requires us to set an overall scale in physical units in our lattice calculations, and this is done using the string tension. One might question how reliable is this procedure. There are various reasons to believe that it is certainly correct to within ±50%. For example the value of the non-perturbative $\langle \alpha_s F_{\mu\nu} F_{\mu\nu} \rangle$ as measured on the lattice [16] agrees with the expectations of the QCD sum rules [18] [‡6] – a change of the mass scale by a factor of ~3–4 [as required if we want to satisfy (1)] would be unacceptable. The diameter of the glueballs [15,16] would shrink to ~0.15 fm under such a rescaling – and their masses would become hopelessly large; as would the masses of mesons and baryons (albeit according to preliminary calculations in the quenched approximation [‡7]).

The serious violation of (1) and the lack of topological structure suggests that the topological charge density may approach the continuum limit more slowly than the string tension or glueball spectrum. It is interesting then to compare quantitatively our results for the 8^4 lattice with those of ref. [12] on a 4^4 lattice. To do so requires a subtraction of the perturbative piece of $\langle (\Sigma F\tilde{F})^2 \rangle$, and for this purpose we shall use the results of ref. [12]. To facilitate comparisons we introduce the quantity

$$A = \frac{1}{\mathrm{VT}} \left\langle \left(\frac{g^2}{16\pi^2 N} \int \mathrm{d}^4 x \, F\tilde{F}(x) \right)^2 \right\rangle , \tag{9}$$

and the combination

$$I = \pi^4 2^{18} a^4 A , \tag{10}$$

as used in ref. [12]. The perturbative piece, I_{PT}, for a 4^4 lattice is (for $F\tilde{F}_{\mathrm{B}}$) [12]

$$I_{\mathrm{PT}}|_{4^4} \simeq 702 . \tag{11}$$

[‡6] The most recent analysis following the method of ref. [18] is given in ref. [19] and leads to $\langle (\alpha_s/\pi) F_{\mu\nu} F_{\mu\nu} \rangle \approx (275\ \mathrm{MeV})^4$. A more recent analysis involving the $\langle F_{\mu\nu}^3 \rangle$ piece [20] and potential model arguments [21] agree on a value closer to $\langle (\alpha_s/\pi) F_{\mu\nu} F_{\mu\nu} \rangle \approx (390\ \mathrm{MeV})^4$. In a lattice calculation [16] in SU(2), using the same scale as in the present paper we find $\langle (\alpha_s/\pi) F_{\mu\nu} F_{\mu\nu} \rangle = (325 \pm 5\ \mathrm{MeV})^4$, which suggests that our scale is good to about ±25%. We thank S. Narison for making us aware of the current status of the work in QCD sum rules, and for emphasizing the reliability of $\langle \alpha_s F_{\mu\nu} F_{\mu\nu} \rangle$ as a means of setting the scale on the lattice in physical units.

[‡7] For a recent review see ref. [22].

To obtain the value for an 8^4 lattice we extrapolate using the data in ref. [12] for the lattice size dependence of the calculated piece of the $F\tilde{F}_{\mathrm{A}}$ operator. The size dependence is in fact very small and we estimate

$$I_{\mathrm{PT}}|_{8^4} \simeq 735 \pm 5 . \tag{12}$$

Subtracting this from our data for I, we can compare the non-perturbative pieces, I_{NPT}, for our 8^4 lattice with that of ref. [12] for a 4^4 lattice:

$$I_{\mathrm{NPT}}|_{8^4} / I_{\mathrm{NPT}}|_{4^4} = 1.97 \pm 0.21 . \tag{13}$$

We see strong finite size effects. [The error in (13) is mainly statistical; we emphasize that the uncertainty in extrapolating the perturbative piece from a 4^4 to an 8^4 lattice is negligible on the scale of the number in (13).]

We now compare our 4^4 lattice embedded in the 8^4 lattice with the 4^4 lattice with periodic boundary conditions [12]. We take the perturbative piece to be

$$I_{\mathrm{PT}}|_{4^4 \in 8^4} = 702 \pm 35 , \tag{14}$$

where we have taken a large enough uncertainty to cover any possible change in I_{PT} when we change boundary conditions (we know that $I_{\mathrm{PT}}|_{4^4 \in 8^4} \leqslant I_{\mathrm{PT}}|_{8^4}$). We find

$$I_{\mathrm{NPT}}|_{4^4 \in 8^4} / I_{\mathrm{NPT}}|_{4^4} = 2.11 \pm 0.23 . \tag{15}$$

Hence $\langle (\Sigma F\tilde{F})^2 \rangle$ not only possesses strong finite size effects, but also depends strongly on boundary conditions.

Our above results indicate that for $\beta \sim 2.3$ [$\beta \sim 5.7$ for SU(3)] the topological charge density is still distant from its continuum limit. This is reassuring since it leaves open the possibility that the theory may eventually display a topological structure and may satisfy (1). One may wonder how this fits in with the apparent renormalisation group behaviour found in ref. [12] in the region $2.2 \lesssim \beta \lesssim 2.4$ which straddles our coupling. The errors of the data in ref. [12] are perhaps large enough that it is not too improbable for this behaviour to be accidental.

Can we understand our negative findings? First let us specify the requirements a lattice should satisfy if it is to embody accurately some non-perturbative physics characterized by a length ξ. Let the lattice have a spatial extent of $L_s a$ and a temporal extent of

$L_t a$. In order for the lattice to be large enough to contain the fluctuations of interest, and in order for it to be fine-grained enough not to distort the physics of interest, we require

$$\min(\tfrac{1}{2}L_s a, \tfrac{1}{2}L_t a) \gg \xi \gg a \,, \qquad (16)$$

where the factor of $\frac{1}{2}$ comes because of the periodic boundary conditions. In order for the physical temperature of the lattice to be below the deconfining phase transition [23] we also require

$$\text{Temperature} \equiv 1/L_t a \ll 200 \text{ MeV} \,. \qquad (17)$$

A further useful input is the diameter, l_G, of the typical low-lying glueball, which is [16]

$$l_G \approx (1.5\text{–}2)\, a(\beta = 2.3) \,. \qquad (18)$$

Consider now eq. (1) in the light of (16), (17). We may take l_G to represent the size of typical non-perturbative fluctuations relevant to hadronic structure, $\xi \approx l_G$. Then even with weak rather than strong inequalities in (16), (17), we see that a 4^4 lattice can only hope to represent physics in a narrow window around $\beta \approx 2.2$ – by $\beta \approx 2.3$ it is already at a temperature of ~230 MeV. This shows that it is dangerous to use a 4^4 lattice for an analysis of eq. (1). An 8^4 lattice on the other hand has a "window of physics" that is reasonably large: $2.2 \lesssim \beta \lesssim 2.5$. The same size window will, of course, hold for a 4^4 lattice embedded in the 8^4 lattice. So we might have hoped to obtain a reasonable value on our 8^4, or embedded 4^4 lattices. That we have not *may* have to with the fact that the characteristic mass in the $F\tilde{F}$ channel, the lowest lying 0^- glueball, is heavier than the 0^+ glueball:

$$1/m(0^-) \approx 1/m(0^+) \approx a(\beta = 2.3) \,. \qquad (19)$$

This perhaps indicates that $\xi \sim a$ rather than $2a$, in which case we would have to go to $\beta \gtrsim 2.5$ to truly test (1), and a lattice larger than 8^4 would be desirable.

Let us now turn to the observed absence of instantons. This is easier to understand. Instantons, being semiclassical constructs, are only "reliably" expected to appear on size scales smaller than l_G (which characterizes the size scale of complex and not well understood non-perturbative fluctuations). On the other hand we note that instantons are not topologically stable on a coarse lattice: the region of non-trivial energy density, which in the continuum limit is forced onto us by continuity, can, on a lattice, slip through in between lattice sites, partially or wholly. For a small enough lattice spacing instantons should appear on the lattice for the same reason they do in the continuum theory: the entropy wins over the action. For this to happen the lattice must be sufficiently fine-grained that the number of states for which a typical instanton slips significantly between lattice sites is overwhelmed by the number of states in which the instanton is trapped on the links. This requires

$$l_G \gtrsim \rho \gg a \,, \qquad (20)$$

where ρ is a typical instanton size. Since small instantons are suppressed as $\exp[-8\pi^2/g^2(\rho)]$ the interesting range of ρ will be close to l_G. We may thus hope to see a signal of the topological structure, if we go to, say, $\beta \gtrsim 2.6$. This is a conclusion similar to that of the previous paragraph. This may be no accident: for SU(2) and SU(3) $\langle(\Sigma F\tilde{F})^2\rangle$ may indeed be dominated by instanton contributions.

We can understand now why our search for topological structure at $\beta = 2.3$ [or $\beta = 5.7$ in SU(3)] was too optimistic. We have also shed some understanding on the apparent failure of eq. (1). Our analysis suggests that the best strategy in resolving these questions is to use a sublattice of a lattice large enough to be useful for $\beta \gtrsim 2.6$. On the question of instantons SU(2) is as good as SU(3), because instantons are SU(2) objects and they arise in SU(3) through various embeddings of SU(2) in SU(3).

Beyond the above basically kinematic, observations one may, more fundamentally, question the appropriateness of the $F\tilde{F}$ operators used herein. It turns out [24] that there are some subtle difficulties. These questions, and measurements deeper in the continuum limit, will appear elsewhere [24].

In summary: We have calculated $\langle(\Sigma F\tilde{F})^2\rangle$ in both SU(2) and SU(3). Our SU(2) calculations were on a large 8^4 lattice and on a 4^4 sublattice embedded in this 8^4 lattice (thus freeing us from the periodic boundary condition constraint). Our numerical results were as dismally small (roughly) as those of ref. [12] for SU(2) on a small 4^4 lattice. At a more detailed level we find that working on a 8^4 lattice, or on the embedded 4^4 lattice, doubles the "non-perturbative" piece of $\langle(\Sigma F\tilde{F})^2\rangle$. This certainly indicates a lack of scaling – and possibly a problem with periodic boundary conditions. We establish criteria for where scaling might set in. We also search for instantons (the first such calculation we are aware of). We find ni signal in either SU(2) or SU(3), on any of our lattices. We clarify why this is so and establish criteria for how to do better. Work is in progress on these and related questions [24].

A belated scaling of physics involving the topological charge density would have obvious and important consequences for the calculation of the spectrum of mesons and baryons: both in the U(1) sector of mesons, and also more generally if instantons play an important role in chiral symmetry breaking.

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