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Addendum

PRELIMINARY EVIDENCE FOR $U_A(1)$ BREAKING IN QCD
FROM LATTICE CALCULATIONS

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Reference 21) is incomplete. It should read :

- 21) B. Berg and M. Lüscher, Nucl.Phys. B190 (1981) 412 ;
M. Lüscher, Bern Preprint BUTP-4/1981 ;
G. Martinelli, R. Petronzio and M.A. Virasoro, CERN Preprint TH. 3076 (1981).

Note added

After completion of this work we received a paper by M. Lüscher (Bern Preprint PUTP-4/1981) in which a new definition of the topological charge density on a four-dimensional lattice is given. Such a definition leads to a quantized topological charge and therefore does not suffer from perturbative contributions.

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ABSTRACT

We suggest a simple definition of the topological charge density $Q(x)$ in the lattice Yang-Mills theory and evaluate $A \equiv \int d^4x \langle Q(x) Q(0) \rangle$ in $SU(2)$ by Monte Carlo simulation. The "data" interpolate well between the strong and weak coupling expansions, which we compute to order g^{-12} and g^6 respectively. After subtraction of the perturbative tail, our points exhibit the expected asymptotic freedom behaviour giving $A^{1/4} \approx (0.11 \pm 0.02)K^{1/2}$, K being the $SU(2)$ quarkless string tension. Although a larger value for $A^{1/4}K^{-1/2}$ would be preferable, we are led to conclude (at least tentatively) that the $U_A(1)$ problem of QCD is indeed solved perturbatively in the quark loop expansion.

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1. INTRODUCTION

In the last couple of years the idea¹⁾ that a non-trivial topological charge in quantum chromodynamics (QCD) can solve its $U(1)$ problem [i.e., explicitly break the $U(1)$ axial symmetry] has been made more precise and quantitative^{2),3)} through the use of expansions of the $1/N$ type. The situation, which can be summarized in terms of a simple effective Lagrangian⁴⁾, is as follows:

- i) in massless QCD, at the one-quark loop level (or, alternatively, at leading order in $1/N_{\text{colour}}$), a set of L^2 unmixed Goldstone bosons π_{ij} ($i, j = u, d, s, \dots$) occurs as a result of the spontaneous breaking^{*)} of $U(L) \otimes U(L)$ chiral symmetry down to $U(L)_{\text{vector}}$ (L is the number of massless flavours);
- ii) the strong axial anomaly equation:

$$\partial_\mu J_{\mu 5}^{(x)} \equiv \partial_\mu \sum_{i=1}^L \bar{\Psi}_i \gamma_\mu \gamma_5 \Psi_i = 2L Q(x) \quad (1.1)$$

$$Q(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a F_{\rho\sigma}^a \quad (1.2)$$

implies that, at the two-loop (OZI violating) level, the pseudoscalar mass matrix in the flavourless sector is non-zero. The matrix element between π_{ii} and π_{jj} is given by:

$$M_{ij}^2 = 2 F_\pi^{-2} A \quad i, j = 1 \dots L \quad (1.3)$$

with $F_\pi \approx 95$ MeV the pion decay constant and, in Euclidean space:

$$A = \int d^4x \langle 0 | Q(x) Q(0) | 0 \rangle \Big|_{\text{no quarks}} \quad (1.4)$$

In order to estimate A from the actual pseudoscalar spectrum, one has to add to M_{ij}^2 the standard current algebra contribution coming from non-zero (but small) quarks masses. One thus obtains^{3),7)} the relation (for $L = 3$):

*) Several arguments for the necessity of such breaking have been given under different (reasonable) assumptions^{5),6)}.

$$\frac{2LA}{F_\pi^2} = (m_\eta^2 + m_{\eta'}^2 - 2m_K^2)_{\text{exp.}} = 0.726 \text{ GeV}^2 \quad (1.5)$$

$$A \simeq (180 \text{ MeV})^4$$

The resolution of the $U_A(1)$ problem, as well as a successful description of the dynamics of the pseudoscalar nonet, is thus reduced to explain why $A \neq 0$ in the quarkless theory^{*}) although it vanishes to all orders in perturbation theory.

From general arguments⁸⁾, $Q(x)$ and A are expected to be renormalization group invariant, in agreement with their relationship with physical masses. This implies that the dependence of A upon the subtraction point μ and the coupling constant g is of the form:

$$A = c \left[\mu \exp \left(\int_g dg' / \beta(g') \right) \right]^4 \approx c \left[\mu (-\beta_0 g^2)^{\beta_1/2\beta_0^2} \exp \left(\frac{1}{2\beta_0 g^2} \right) \right]^4 \quad (1.6)$$

where $\beta(g) \simeq \beta_0 g^3 + \beta_1 g^5 + O(g^7)$ and

$$\beta_0 = -\frac{11}{3} \frac{N}{16\pi^2}, \quad \beta_1 = -\frac{34}{3} \left(\frac{N}{16\pi^2} \right)^2 \quad (1.7)$$

in the quarkless $SU(N)$ gauge theory. The dimensionless quantity c is what we would like to compute. At present the only techniques available for computing dimensional quantities like A are those provided by first regulating the theory on a lattice and then by performing either strong coupling expansions⁹⁾⁻¹¹⁾ or numerical Monte Carlo simulations^{12),13)}.

In this paper we present, for the case of $SU(2)$, a first indication that the renormalization group behaviour (1.6) with a non-zero (positive) value of c emerges from lattice calculations. The result is obtained using a simple minded (but, we think, attractive) definition of $Q(x)$ on the lattice. The idea is, of course, that in the physical continuum limit ($a \rightarrow 0$), any definition with the correct naive $a \rightarrow 0$ limit should give the same result.

^{*}) It was argued⁶⁾ by one of us, (G.V.), that even the spontaneous breaking of chiral symmetry in QCD follows from $A \neq 0$.

What is relevant is, as usual, the ratio of $A^{1/4}$ to another physical parameter with dimensions of a mass. Comparing our curves with those of Creutz¹³⁾, we extract:

$$A^{1/4} = (0.11 \pm 0.02) K^{1/2} \quad (1.8)$$

where K is the $SU(2)$ quarkless string tension. If one takes for K the value $(2\pi\alpha')^{-1}$ of the dual string model with $\alpha' = 0.9 \text{ GeV}^{-2}$, then one obtains

$$A^{SU(2)} \simeq (45 \pm 10 \text{ MeV})^4 \quad (1.9)$$

i.e., a rather small number compared to the desired value (1.5). On the other hand, assuming that $A^{1/4} K^{-1/2}_{\text{no quarks}}$ varies little from $SU(2)$ to $SU(3)$ (as suggested by $1/N$ expansion considerations) and using the known relation¹¹⁾ between $K^{1/2}$ and Λ_{MOM} in $SU(3)$, one would get

$$A^{SU(3)} \simeq \left(0.26 \Lambda_{\text{MOM}}^{SU(3)} \right)^4 \quad (1.10)$$

which is much more acceptable. A discussion of this numerology will be given at the end of Section 5.

The outline of the paper is as follows. In Section 2 we discuss some possible definitions of $Q(x)$ in the lattice, showing that they all suffer from a non-zero perturbative expansion in g (even at zero momentum). In Section 3 we compute the first non-trivial term in the perturbative expansion of A , adopting for $Q(x)$ a definition which appears most suitable for joining the strong coupling behaviour with the asymptotic freedom regime. In Section 4 we describe our strong coupling calculations up to order $(1/g^2)^6$, improved by character expansion techniques¹⁰⁾. In Section 5 we present the output of our Monte Carlo simulation and we discuss the subtraction of the perturbative tail. We then show the emergence of the expected behaviour (1.6) in a region of the weak coupling regime and, finally, we extract and discuss the numerical relations (1.8) and (1.10). An outline of future investigations is given in Section 6.

2. DEFINITIONS OF $Q(x)$ ON THE LATTICE

A rather natural definition of $Q(x)$ on the lattice was given sometime ago by Peskin¹⁵⁾ on the basis of the well-known property⁹⁾ of the product of four link variables around one plaquette of side a :

$$U_{n,\mu\nu} \equiv U_{n,\mu} U_{n+\mu,\nu} U_{n+\mu,\nu}^+ U_{n,\mu}^+ \equiv \exp \left\{ i \sum_b \frac{g}{\sqrt{2}} F_{\mu\nu,n}^b T^b \right\} \quad (2.1)$$

$$F_{\mu\nu,n}^b \xrightarrow{a \rightarrow 0} g a^2 F_{\mu\nu}^b(x_n) + O(a^3)$$

where T^b are the generators of the gauge group and $F_{\mu\nu}^b$ is the usual field strength tensor. In the same way as one obtains from (2.1) the Yang-Mills action as:

$$\sum_{n,\mu\nu} \text{Tr} (U_{n,\mu\nu} - 1) \xrightarrow{a \rightarrow 0} -\frac{1}{4} g^2 a^4 F_{\mu\nu}^b F_{\mu\nu}^b + O(a^5) \quad (2.2)$$

one also finds:

$$Q_n^{(P)} \equiv - \frac{\epsilon_{\mu\nu\rho\sigma}}{32\pi^2} \text{Tr} [U_{n,\mu\nu} U_{n,\rho\sigma}] \xrightarrow{a \rightarrow 0} a^4 Q(x_n) + O(a^5) \quad (2.3)$$

We see that $Q_n^{(P)}$ is a sum of eight link Wilson loops of the type shown in Fig. 1. Moreover, because of the $\epsilon_{\mu\nu\rho\sigma}$ tensor, $Q^{(P)}$ contains links in everyone of the four space-time directions. On the other hand, this definition does not symmetrically treat the positive and negative directions of each axis and this prevents $Q^{(P)}$ from having definite parity. The problem is easily overcome by the symmetrized definition^{*)}

$$Q_n^{(S)} \equiv - \sum_{(\mu,\nu,\rho,\sigma)=\pm 1}^{\pm 4} \frac{\tilde{\epsilon}_{\mu\nu\rho\sigma}}{2^4 32\pi^2} \text{Tr} [U_{n,\mu\nu} U_{n,\rho\sigma}] \quad (2.4)$$

with $1 = \tilde{\epsilon}_{1234} = -\tilde{\epsilon}_{2134} = -\tilde{\epsilon}_{-1234}$ etc., which has the same naive $a \rightarrow 0$ limit as $Q_n^{(P)}$. Equations (2.3) and (2.4) then imply that our quantity A is given by

$$A \xrightarrow{a \rightarrow 0} 1/a^4 \sum_n \langle 0 | Q_n^{(S)} Q_0^{(S)} | 0 \rangle \equiv A_L^{(S)} \quad (2.5)$$

in the naive continuum limit.

*) We are grateful to P. Hasenfratz for very constructive remarks on this point.

An alternative, more natural, definition of Q on the lattice can be obtained by first realizing that the Wilson loop of Fig. 1 consists of two orthogonal plaquettes lying on the elementary hypercube of Fig. 2. The latter contains eight three dimensional cubes, 24 plaquettes, 32 links and 16 vertices labelled in Fig. 2 so that labels of opposite vertices differ by eight. A typical loop in the definition (2.5) is then $(1,2,3,4,1,5,6,2,1)$ with the point 1 assuming a privileged role with respect to the other six points.

A definition of Q treating all the 16 vertices symmetrically is:

$$Q_n = - \frac{1}{64\pi^2} \sum_{i=1}^{48} W_n(P_i) (-1)^{\pi_i} \quad (2.6)$$

where n is now a hypercube (not a site) label and $W_n(P_i)$ is the Wilson loop operator for the i^{th} closed path P_i on the n^{th} hypercube. A generic P_i starts from one of the 16 vertices, goes in four steps to the opposite vertex in any possible way and comes back in the same (now unique) order. There are $4! \times 16/8 = 48$ inequivalent oriented paths. Examples of P_i are $P_0 = (1,2,3,7,9,10,11,15)$; $P_1 = (1,2,6,7,9,10,14,15)$ etc. The 48 paths will be classified better in Section 4. Obviously, all the eight vertices of P_i are treated symmetrically and the same is true for positive and negative directions along each axis. Hence the definition (2.6) has automatically the correct parity property provided the signs $(-1)^{\pi_i}$ are defined in agreement with the $\tilde{\epsilon}$ symbol of Eq. (2.5) (+1 for P_0 , -1 for P_1 etc). An alternative way to write (2.6) is then:

$$Q_n = - \frac{1}{2^4 32\pi^2} \sum_{(\mu,\nu,\rho,\sigma)=\pm 1}^{\pm 4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \text{Tr} \left[U_{n,\mu} U_{n+\mu,\nu} U_{n+\mu+\nu,\rho} \times \right. \\ \left. \times U_{n+\mu+\nu+\rho,\sigma} U_{n+\nu+\rho+\sigma,\mu}^+ U_{n+\rho+\sigma,\nu}^+ U_{n+\sigma,\rho}^+ U_{n,\sigma}^+ \right] \quad (2.7)$$

With either definition one still has:

$$A \xrightarrow{a \rightarrow 0} \frac{1}{a^4} \sum_n \langle 0 | Q_n Q_0 | 0 \rangle \equiv A_L \quad (2.8)$$

We have found the second definition [(2.6) or (2.7)] to be preferable to (2.5) on several accounts: i) the strong coupling expansion of $A_L^{(S)}$ is more complicated than the one of A_L because it contains, from the start, plaquettes in the definition of $Q_n^{(S)}$; ii) while the strong coupling expansion of A_L starts alternating in sign (see Section 4) and shows a clear tendency to bend down at

values of $\beta = 4/g^2$ around 2, $A_L^{(S)}$ starts from a lower value at $\beta = 0$ and appears to be flattish at small β . This presumably means the need for many terms in the strong coupling series before the expected turnover begins to appear;

iii) Monte Carlo calculations are more time consuming with the first definition because of its smaller symmetry. For these reasons we stick to the second definition (2.6) in this first exploratory study.

A common feature of the lattice versions of local operators is that their expectations values are non-zero in perturbation theory. A typical case¹⁶⁾ is the expectation value of the plaquette which, in the naive continuum limit, is related to the expectation value of $g^2 F_{\mu\nu}^a F_{\mu\nu}^a$ [see Eq. (2.2)]. This latter quantity is set to zero in continuum perturbation theory as any other physical dimensional quantity, while one finds¹⁶⁾ that the perturbative ($\beta \rightarrow \infty$) tail of the plaquette is quite sizeable with respect to the physically relevant non-perturbative part even near the turnover point ($\beta \sim 2$). One could have hoped that this problem would not arise for the operator $\int d^4x Q(x)$ which vanishes automatically in perturbation theory, $Q(x)$ being a total divergence. This is not the case, however, for either one of our definitions of Q_L , since in a small g expansion of Q_L operators of arbitrarily high dimension which are not total divergences do occur. Although they appear in the expansion multiplied by correspondingly high powers of a , their matrix elements diverge for $a \rightarrow 0$ precisely as required by naive dimensional counting so that their perturbative contributions are all of the same order in a .

As in Ref. 16), the attitude that we shall take here is that, for each operator of dimension higher than 4, once the perturbative contribution has been subtracted out, the remainder should behave as $\exp(-\gamma/g^2)$ as $g^2 \rightarrow 0$ with a coefficient γ larger than that of the (lowest dimension) operator which survives in the naive $a \rightarrow 0$ limit. Unless this is the case, the possibility of extracting renormalization group invariant quantities such as A or $\langle g^2 F^2 \rangle$ from lattice calculations appears to be hopeless. In this respect, the results obtained for $\langle g^2 F^2 \rangle$ in Refs. 16) and 17) are certainly encouraging.

3. THE WEAK COUPLING EXPANSION OF A_L

We have already stated that the weak coupling expansion of A_L , as given by Eq. (2.8), is non-vanishing. In order to see how this happens, consider, for instance, the weak coupling expansion^{*)} of the quantity $Q_n^{(P)}$ defined in Eq. (2.3). Defining as usual

*) We are very grateful to P. Hasenfratz for having initiated us to the techniques of weak coupling lattice calculations.

$$U_{n,\mu} \equiv \exp(iga A_{n,\mu}^b T^b) \quad (3.1)$$

one finds:

$$Q_n^{(P)} = \frac{g^4}{64\pi^2} \varepsilon_{\mu\nu\rho\sigma} \Delta_\mu A_{n,\nu}^b \Delta_\rho A_{n,\sigma}^b + O(g^3) \quad (3.2)$$

where Δ_μ is the finite difference operator

$$\Delta_\mu f_n = (f_{n+\mu} - f_n)/a \quad (3.3)$$

Going over to momentum space, one obviously has:

$$\Delta_\mu \xrightarrow{\text{F.T.}} (e^{-iP_\mu a} - 1)/a \xrightarrow{a \rightarrow 0} -iP_\mu + O(aP_\mu^2) \quad (3.4)$$

One can then check that, to this order, $Q_n^{(P)}$ acts as a two gluon vertex of the form:

$$\frac{Q^{(P)}(k)}{a^4} \sim g^2 \varepsilon_{\mu\nu\rho\sigma} \int_{-\pi/a}^{\pi/a} d^4p d^4q \delta^{(4)}(k+p+q) \frac{(e^{-ip_\mu a} - 1)(e^{-iq_\nu a} - 1)}{a^2} A_{\mu}^c(-p) A_{\nu}^c(-q) \quad (3.5)$$

Clearly this expression is not vanishing at $k = 0$ ($p = -q$) except in the limit $a \rightarrow 0$. Inserting the expression (3.5) in the definition of $A_L^{(P)}$ Eq. (2.4), one immediately finds a non-zero contribution to this quantity at order g^4 . One checks, however, that with the symmetrized expression (2.6) the two gluon vertex itself goes to zero at $k = 0$. Unfortunately, this result does not persist to higher orders in g . In this respect, the definition (2.6) of Q_n , which we adopt in the following, behaves in the same way as the definition (2.4). A straightforward, but lengthy and tedious calculation gives the following result for the first non-trivial contribution to A_L in the $SU(2)$ case

$$\pi^4 2^{18} a^4 A_L = c_3 \beta^{-3} + O(\beta^{-4}) = c_3 (g^2/4)^3 + O(g^2) \quad (3.6)$$

$$\begin{aligned}
 C_3 = & 3 \cdot 2^9 \int_{-\pi}^{+\pi} \frac{d^4 k}{(2\pi)^4} \int_{-\pi}^{+\pi} \frac{d^4 p}{(2\pi)^4} \int_{-\pi}^{\pi} d^4 q \delta^{(4)}(k+p+q) \sum_{\mu\nu\rho\sigma} \varepsilon_{\mu\nu\rho\sigma} \varepsilon_{\mu\nu\rho\sigma} \\
 & \cdot \left[\sum_{\alpha} (1 - \cos k_{\alpha}) \cdot \sum_{\beta} (1 - \cos q_{\beta}) \cdot \sum_{\gamma} (1 - \cos p_{\gamma}) \right]^{-1} \cdot \\
 & \cdot \left\{ \frac{1}{3} \left[C_{\mu} (e^{-ik_{\sigma}} + e^{-iq_{\sigma}}) (e^{-ip_{\nu}} + e^{-ip_{\rho}}) (e^{-ik_{\rho}} + e^{-ip_{\sigma}}) + \right. \right. \\
 & + \sin k_{\mu} (1 + e^{ik_{\nu}}) \left[(1 + e^{ip_{\sigma}}) (e^{-ik_{\rho}} + e^{-ip_{\sigma}}) + (1 + e^{iq_{\rho}}) (e^{-iq_{\sigma}} - ik_{\sigma}) \right]_{\text{cont.}}^{(3.6)} \\
 & + \sin q_{\mu} (1 + e^{iq_{\rho}}) \left[(1 + e^{ik_{\nu}}) (e^{-ik_{\sigma}} + e^{-iq_{\sigma}}) + (1 + e^{ip_{\sigma}}) (e^{-ip_{\nu}} + e^{-iq_{\nu}}) \right] \\
 & + \sin p_{\mu} (1 + e^{ip_{\sigma}}) \left[(1 + e^{iq_{\rho}}) (e^{-ip_{\nu}} + e^{-ip_{\rho}}) + (1 + e^{ik_{\nu}}) (e^{-ik_{\rho}} + e^{-ip_{\sigma}}) \right] \Bigg]^2 + \\
 & \left. + 16 (1 - \cos k_{\sigma}) [1 + \cos(q_{\nu} - p_{\nu})] \sin p_{\mu} \sin q_{\rho} [\sin p_{\mu} \sin q_{\rho} - \sin p_{\rho} \sin q_{\mu}] \right\}
 \end{aligned}$$

where

$$C_{\mu} = \sin k_{\mu} + \sin p_{\mu} + \sin q_{\mu} \quad (3.7)$$

The length of Eq. (3.6) is a clear indication that going beyond this order may prove to be an impossible task. In Table 1 we give the numerical result for C_3 of Eq. (3.6) for the case of a finite lattice of sizes 3^4 to 5^4 as well as for the case of an infinite lattice. Notice that the finite lattice results do not differ by more than 15% from that of the infinite lattice. For the case of $SU(N)$, the values of Table 1 have to be multiplied by the factor $N(N^2-1)/6$. As already discussed in Section 2, we shall use this result to make a subtraction on our Monte Carlo data for A_L (see Section 5).

4. STRONG COUPLING EXPANSION OF A_L

Following standard techniques⁹⁾⁻¹¹⁾, we have performed a strong coupling expansion of A_L , as defined by Eqs. (2.6) and (2.8) up to order g^{-12} . The lowest order terms in $1/g^2$ come from picking up the term with $n = 0$ in the

sum over n of Eq. (2.8) so that the paths appearing in Q_0 and Q_n through Eq. (2.6) lie on the same hypercube. Since we can arbitrarily choose the path in Q_0 to be $P_0 = (1,2,3,7,9,10,11,15)$ (and gain a factor 48) we shall have

$$a^4 A_L = 48 \cdot \left(\frac{1}{64\pi^2} \right)^2 \sum_{i=1}^{48} (-1)^{\pi_0 + \pi_i} \langle W_0(P_i) W_0(P_0) \rangle + (n \neq 0) \quad (4.1)$$

Evaluation of (4.1) can be done by first classifying each of the 48 paths P_i with respect to P_0 . One finds that the 24 distinct (unoriented) paths can be subdivided as follows:

- i) P_0 itself;
- ii) four paths like $(1,2,6,7,9,10,14,15)$ which share with P_0 six vertices and four links;
- iii) eight paths like $(1,2,6,12,9, \text{etc.})$ and
- iv) four paths like $(1,2,16,12,9, \text{etc.})$ both sharing with P_0 four vertices and two links;
- v) two paths like $(1,4,14,13,9, \text{etc.})$ with four vertices in common with P_0 ;
- vi) four paths like $(1,4,14,13,9, \text{etc.})$ with just two vertices in common with P_0 and finally
- vii) one path with $(4,8,5,6,12,16,13,14)$ with no vertex in common with P_0 .

Each one of the above 24 paths can be taken in either direction. In the $SU(2)$ case the orientation of the path does not matter and from now on we shall restrict ourselves to this case.

The systematics of the strong coupling expansion is made easier by the use of the character expansion technique¹⁰⁾. For $SU(2)$, and up to the order β^6 at which we work, it is enough to use the formula

$$\exp \left(\beta/4 \operatorname{Tr}(U+U^+) \right) = 1 + \bar{\beta}/4 \operatorname{Tr}(U+U^+) + \dots \quad (4.2)$$

where $\bar{\beta}/4$ is the coefficient of the fundamental representation (spin 1/2) character and the dots indicate characters in higher spin representations of $SU(2)$. One finds

$$\bar{\beta} = 4 I_2(\beta) / I_1(\beta) = \beta \left(1 - \beta^2/24 + \beta^4/384 + \dots \right) \quad (4.3)$$

with $I_n(\beta)$ the usual modified Bessel function. We have checked that, to $O(\beta^6)$, higher spin characters do not contribute to A_L . Also, as far as we could check,

the contributions $O(\beta^6)$ coming from terms with $n \neq 0$ in Eq. (2.8) (surprisingly) cancel out leaving us with the evaluation of (4.1). Now, for P_i in each of the seven classes described above, we have different strong coupling contributions. The leading contribution as $\beta \rightarrow 0$ comes from $P_i = P_0$. Since the group integrals (contractions) give just one we get:

$$A_L \xrightarrow{\beta \rightarrow 0} \frac{1}{a^4} (48) \left(\frac{1}{\sqrt{4\pi^2}} \right)^2 \cdot 2 = \frac{3}{2^7 \pi^4} \frac{1}{a^4} \equiv A_L^\infty \quad (4.4)$$

where the factor of two comes from the two orientations of P_0 and would be absent for $SU(N)$, $N > 2$. In a similar way, since $\text{Tr} U = \text{Tr} U^\dagger$ for $SU(2)$, the effective coefficient of the spin 1/2 character in Eq. (4.2) is $\bar{\beta}/2$ rather than $\bar{\beta}/4$. At order $\bar{\beta}^2$, we get contributions from P_i in the class ii) (described above) if we use twice the action expanded as in (4.2). Taking into account that there are four paths in this class, that the relative sign of P_i and P_0 is -1 and that the group integrals give $(1/2)^2$, one gets a contribution

$$A_L^\infty \times 4 \times (-1) \times (\bar{\beta}/2)^2 \times (1/2)^2 = -\bar{\beta}^2/4 A_L^\infty \quad (4.5)$$

In a similar way, the ten paths of classes iii) and v) give

$$A_L^\infty \times 10 \times (+1) \times (\bar{\beta}/2)^4 \times (1/2)^4 = \frac{5}{2^7} \bar{\beta}^4 A_L^\infty \quad (4.6)$$

For the contribution of order $\bar{\beta}^6$ the situation starts to get complicated. The paths in classes iv) and vi) are found to give a contribution

$$A_L^\infty \times 28 \times (-1) \times (\bar{\beta}/2)^6 \times (1/2)^6 = -\frac{7}{2^{10}} \bar{\beta}^6 A_L^\infty \quad (4.7)$$

There are, however, two sorts of new contributions to this order. One stems from the fact that previously found contributions of $O(\bar{\beta}^2)$ can be transformed into contributions of $O(\bar{\beta}^6)$ by replacing a plaquette with five others forming a cube together with the removed original one. Since there are four ways of building such a cube and the extra weight to pay for a cube is $(\bar{\beta}/4)^4$ one can effectively take this "plaquette excitation" contribution into account by the replacement

$$\bar{\beta} \rightarrow \bar{\beta} (1 + \bar{\beta}^4/64) \quad (4.8)$$

There is, however, a related effect due to the fact that one has to divide the strong coupling diagrams for $Q_n Q_0$ by the vacuum diagrams. The first non-trivial vacuum diagram is again a cube and gives

$$\langle 0|0 \rangle = 1 + \sum_{\text{Cubes}} \bar{\beta}^6 / 4^5 + \dots \quad (4.9)$$

Usually vacuum diagrams cancel against disconnected diagrams in the numerator. This does not happen however when the cube has one face in common with a pre-existing plaquette of the connected diagrams. The effect (the so-called excluded volume effect) can be taken approximately into account by a further replacement, leading us to define the new strong coupling expansion variable:

$$\tilde{\beta} \equiv \bar{\beta} \left(1 + \bar{\beta}^4 / 64 (1 - \bar{\beta}^2 / 4) \right) \quad (4.10)$$

In terms of $\tilde{\beta}$, collecting contributions (4.4) to (4.7) we get

$$A_L = A_L^\infty \left(1 - \tilde{\beta}^2 / 4 + 5/2^7 \tilde{\beta}^4 - 7/2^{10} \tilde{\beta}^6 \right) + O(\tilde{\beta}^8) \quad (4.11)$$

$$A_L^\infty \equiv \frac{1}{a^4} \frac{3}{2^7 \pi^4}$$

This is our final result to order β^6 . It includes automatically, through the use of the new variable $\tilde{\beta}$, some higher order effects. In any case, the numerical results would not be much different if we had expressed everything in terms of β and had truncated the series at $O(\beta^6)$. We should point out however that, due to its complicated nature, the calculation of the $O(\beta^6)$ contribution should be rechecked by different techniques. We also feel that going systematically to higher orders already calls for the development and use of a computer programme.

Notice that the terms we computed alternate in sign and that all terms become roughly of the same order for $\beta \approx 2$, i.e., around the point at which the famous turnover of the string tension occurs.

In the next sections the above strong coupling calculations will be compared with the Monte Carlo data.

5. MONTE CARLO SIMULATION AND EVALUATION OF A

Existing Monte Carlo techniques^{12),13)} can be readily used for a numerical evaluation of A_L on a finite lattice. We have used the heat bath method on a 4^4 lattice with periodic boundary conditions (p.b.c.). The quantity actually computed is:

$$a^4 A_L^{MC} = \frac{1}{V} \left\langle \left(\sum_{n \in V} Q_n \right)^2 \right\rangle ; V = 4^4 \quad (5.1)$$

which is equal to $\langle (\sum_{n \in V} Q_n) Q_0 \rangle$ thanks to the discrete translational invariance of the periodic lattice. The use of p.b.c. on the link variables $U_{n,\mu}$ immediately raises the question of whether one can get at all a non-zero result for the volume integral of a quantity which, in the naive continuum limit, approaches a total divergence^{*)}. Upon integration by parts, opposite boundary conditions would seem to cancel against each other thanks to periodicity. The point is, however, that even for $a \rightarrow 0$, Q_n can only be written as a finite difference of a function of the $A_{n,\mu}$ variables defined via Eq. (3.1). Clearly, $A_{n,\mu}$ is not uniquely determined by $U_{n,\mu}$ and periodicity in the U 's does not imply periodicity in the A 's. If we want to write the $a \rightarrow 0$ limit of Q_n as a derivative, we have to impose some sort of continuity on the A 's [e.g., $ga(A_{n,\mu} - A_{n+\nu,\mu}) \ll 1$] or else have a singularity in Q_n . But then it is quite possible that p.b.c. in the U 's plus continuity in the A 's imply some non-periodicity of the A 's and a non-zero value of $\sum_n Q_n$ ^{**)}. The above conclusion fits well with the intuitive expectation that the correlation function $\langle Q_n Q_m \rangle$ should vanish exponentially in the separation between the sites n and m . The characteristic scale is given by the inverse mass of the lightest pseudo-scalar glueball: as long as this is substantially smaller than the size of our lattice, boundary effects on the integrated correlation $\langle \sum_n Q_n Q_0 \rangle$ should be negligible. The finiteness of our lattice then puts a lower limit on the value of g at which one can work. The hope is, of course, that the sought for asymptotic freedom behaviour sets in before this critical value of g is reached.

*) Questions of this type were first raised in Ref. 15).

**) We are grateful to C. Rebbi and M.A. Virasoro for very useful discussions on this point and for communicating to us some unpublished work of theirs in two-dimensional compact QED, where they have found the above phenomenon to occur.

We took Monte Carlo data for a few strong coupling points (mainly for a check) and then mainly for values of β larger than 2. We ran up to 6000 sweeps for fixed β using, as link variables, elements of the full $SU(2)$ group. We made hot and cold starts and checked that equilibrium was reached after a small number of sweeps. Nevertheless, fluctuations were rather large as compared, for instance, with those of the plaquette energy. In Fig. 3, the data $\pi^4 2^{18} a^4 A_L^{MC}$ are presented as a function of $\beta = 4/g^2$ with their statistical errors. Strong and weak coupling curves are also given at various levels of approximation, i.e., to $O(\tilde{\beta}^2)$, $O(\tilde{\beta}^4)$ and $O(\tilde{\beta}^6)$ on the strong coupling side [Eq. (4.11)] and to $O(\beta^{-3})$ on the weak coupling side. The agreement at small β , which persists up to $\beta \approx 1.5 \div 2$, indicates the correct performance of our Monte Carlo programme. At the same time, the calculated $C_3 \beta^{-3}$ term is seen to account for the "measured" values for $\beta \gtrsim 2.5 \div 3$ (see, in particular, the point at $\beta = 4$).

The difference between Monte Carlo and the computed β^{-3} term is shown in Fig. 4. We notice that the difference is small, systematically positive and decreasing at large β . A fit to a C_4/β^4 term in the region $\beta \gtrsim 2.8$ turns out to be possible with the result:

$$a^4 A_L^{MC} \underset{\beta \gtrsim 2.8}{\approx} 5.608 \cdot 10^{-4} \beta^{-3} + 2.14 \cdot 10^{-4} \beta^{-4} \equiv A_L^{Pert.} \quad (5.2)$$

Here, encouraged by the fact that the fit is indeed a good one and that the β^{-4} correction is small, we have assumed higher order perturbative corrections [$O(\beta^{-5})$ etc] to be negligible in the region $2 \leq \beta \leq 3$, in which we are interested.

In Fig. 5 we show, on a logarithmic scale, the difference between $a^4 A_L^{MC}$ and $a^4 A_L^{Pert.}$ [as defined by (5.2)] in the interval $2 \leq \beta \leq 2.8$. Amazingly, the points do lie on a straight line with the expected slope [Eq. (1.6) is the one loop approximation $\beta_1 = 0$] giving

$$A^{Non Pert.} \equiv (A_L^{MC} - A_L^{Pert.}) = a^{-4} \exp\left(-\frac{12\pi^2}{11}(\beta - \beta_A)\right), \quad \beta_A = 1.18 \pm 0.03 \quad (5.3)$$

allowing us to estimate the continuum limit value of A .

Equation (5.3) can indeed be compared with the result of Ref. 12) for the $SU(2)$ string tension K

$$K = a^{-2} \exp\left(-\frac{6\pi^2}{11}(\beta - \beta_K)\right), \quad \beta_K = 2.00 \pm 0.05 \quad (5.4)$$

Equations (5.3) and (5.4) give $A^{1/4} \approx (0.11 \pm 0.02)K^{1/2}$, the result anticipated in Equation (1.8).

Another fit to the subtracted data is possible (and even slightly better) with the two loop asymptotic freedom formulae, Eq. (1.6). Comparing that exercise to a similar fit to $K^{18)}$ one again finds the result (1.8) within the errors. Taking for $\sqrt{K}$ the string model value $\sqrt{1/2\pi\alpha'} = 420$ MeV, the value $A^{1/4} \approx (45 \pm 10)$ MeV is obtained. The smallness of this value, as compared with the phenomenological one [Eq. (1.5)], can be attributed to several reasons:

- i) The ratio $A^{1/4}K^{-1/2}$ is computed in the pure SU(2) gauge theory. Although large N expansion arguments suggest a weak N dependence for this quantity, the SU(3) value could differ appreciably from the SU(2) value.
- ii) While A, according to the arguments of Refs. 3) and 4), has to be computed in the quarkless theory, the physical value of the string tension is probably affected by light quark loops. The effect of these is likely that of decreasing K so that $K_{(\text{no quarks})}^{1/2} > K_{\text{Phys}}^{1/2} \approx 420$ MeV. This will push up our result for A.
- iii) Another way to state our result is to express A through Λ_{MOM} which is perhaps a less quark loop dependent quantity than K. Using the relations between Λ_{lattice} and Λ_{MOM} of continuum QCD obtained in Ref. 14), one then gets:

$$A^{1/4} \Big|_{\text{SU}(2)} \simeq 0.15 \Lambda_{\text{MOM}}^{\text{SU}(2)} \quad (5.5)$$

hence $\Lambda_{\text{MOM}}^{\text{SU}(2)} \approx 1.2$ GeV for $A^{1/4} = 180$ MeV.

- iv) A more favourable result is obtained by assuming $A/K_{\text{no q.}}^2$ to be the same in SU(2) and SU(3). Using again Ref. 14) one then gets:

$$A^{1/4} \Big|_{\text{SU}(3)} \simeq 0.26 \Lambda_{\text{MOM}}^{\text{SU}(3)} \quad (5.6)$$

i.e., a good value of A for $500 \text{ MeV} < \Lambda_{\text{MOM}} < 900 \text{ MeV}$, which we can regard as very reasonable. But, of course, with $\Lambda_{\text{MOM}} = 700$ MeV one also predicts:

$$K^{1/2} \Big|_{\substack{\text{su(3)} \\ \text{no quarks}}} \approx 1.6 \text{ GeV} \quad (5.7)$$

and light quarks have to intervene drastically to reduce $K^{1/2}$ to the "observed" string model value of 420 MeV.

- v) Another possible indication for a "large" value of $K^{1/2}|_{\text{no quarks}}$ is offered by a recent calculation of the mass of the lightest scalar glueball by Münster¹⁹⁾ giving

$$m_{gl.} = (1.8 \pm 0.8) K^{1/2} \quad (5.8)$$

Since we might expect glueballs to be relatively heavy (say around 1.5 to 2 GeV) a large value of $K^{1/2}$ (~ 1 GeV) would be preferred.

- vi) Finally, the recent calculations of $\langle g^2 F^2 \rangle|_{\text{no quarks}}$ fit the phenomenological value if a smaller value of Λ_{MOM} (~ 300 MeV) is used in apparent disagreement with our case. The discrepancy can be explained if one assumes, according to some theoretical arguments given in Ref. 20), that $\langle g^2 F^2 \rangle|_{\text{no quarks}}$ is quite larger than the physical value in the presence of two (or three) light quarks.

In conclusion, although we would have preferred to find a larger value for A/K^2 , we cannot say that we are, as yet, in contradiction with other results and/or with experiments also bearing in mind that several non-trivial current algebra extrapolations have been used in Refs. 3) and 4).

6. OUTLOOK

Although we consider the results presented in this paper to be quite encouraging, much work is certainly still needed before one can claim that the non-perturbative value of A is different from zero and can reliably compute its magnitude.

Some of our limitations are of a theoretical nature, in particular our inability to define a Q_L free of perturbative contributions^{*)}. Others come from the limited statistics of the Monte Carlo data we have been able to collect so far.

*) A definition of topological charge which is free of perturbative contributions has been recently given for some two-dimensional models²¹⁾.

For the future we plan to utilize faster programmes, possibly based on finite subgroups of $SU(2)$ ²²⁾, in order to improve the statistics of our data and to extend our calculations. In particular we would like to explore

- i) effects of finite volume and/or of boundary conditions;
- ii) dependence of the value of A from the lattice definition employed. In particular we plan to check whether the expected asymptotic freedom behaviour also emerges using the definition (2.5). Preliminary results seem to indicate that this is actually the case ²³⁾.

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3^4	$C_3 = 12\,539.6$
4^4	$C_3 = 14321.4$
5^4	$C_3 = 14760.7$
∞^4	$C_3 = 15\,034 \pm 92$

Values of C_3 [Eq. (3.6)] for increasing lattice size. The integral in the last line has been computed by a Monte Carlo method using $1.6 \cdot 10^6$ points.

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FIGURE CAPTIONS

- Figure 1 : Wilson loop appearing in Peskin's original definition¹⁵⁾ of the topological charge density.
- Figure 2 : The elementary hypercube with its 16 vertices, 32 links, 24 plaquettes and eight cubes. Labels of opposite vertices differ by eight.
- Figure 3 : Monte Carlo data for $\pi^4 2^{18} a^4 A_L$ with their statistical error bars are shown together with a partly computed, partly fitted, "perturbative tail". Strong coupling curves at order $\tilde{\beta}^2$ (dashed line), $\tilde{\beta}^4$ (dash dotted line) and $\tilde{\beta}^6$ (solid line) are also shown.
- Figure 4 : Computed $C_3 \beta^{-3}$ perturbative term. Fitted $C_4 \beta^{-4}$ perturbative term.
- Figure 5 : Subtracted Monte Carlo data in the region $2.2 \leq \beta \leq 2.4$ and fit to the asymptotic freedom straight line $-12\pi^2/11 (\beta - 2.76)$.

FIG.1

FIG.2

FIG. 3

FIG. 4

FIG. 5