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THE θ-VACUUM IN SU(2) LATTICE GAUGE THEORY

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Monte Carlo determinations of the distribution of topological charge are used to study properties of the SU(2) pure-gauge θ-vacuum. In particular, we compare the possibility that a phase transition occurs, as θ is varied, to the simple dilute instanton gas picture. For small physical volumes we find no deviation from the dilute instanton gas, but for $z_t > 1.5$ there are deviations that may be statistically significant. For example, for $z_t > 1.5$ the partition function has a zero, and the ratio of the fourth and second moments of the charge distribution changes its value suddenly at $z_t \approx 1.5$.

1. Introduction

One of the characteristic features of SU(N) nonabelian gauge theories is the existence of an integer-valued topological charge [1]

$$Q = -\frac{1}{16\pi^2}\int d^4x \, \mathrm{tr}\{F_{\mu\nu}{}^*F_{\mu\nu}\}, \qquad {}^*F_{\mu\nu} = \tfrac{1}{2}\varepsilon_{\mu\nu\rho\sigma}F_{\rho\sigma}. \tag{1.1}$$

This results in an additional term in the QCD action

$$S_\theta = S + i\theta Q, \tag{1.2}$$

which does not modify the classical equations of motion, although there are physical consequences through quantum effects. In particular, each angle $\theta \in [0, 2\pi)$ corre-

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sponds to a different vacuum state, which means that θ is a free parameter*. The appearance of θ has at least three interesting implications.

The vacuum is an eigenstate of CP (and T) only for $\theta = 0, \pi$. Measurements of the electric-dipole moment of the neutron [2, 3] provide a peculiarly small experimental upper bound of $\theta \leqslant 10^{-9}$. Many have sought an explanation for the strong CP-problem, "Why is θ so small?" A popular mechanism introduces an additional U(1) "Peccei–Quinn" symmetry [4] into the standard model. This tunes θ to zero. However, the Peccei–Quinn symmetry must be spontaneously broken [5], and the associated pseudo-Goldstone boson, the axion, has not been observed, despite strenuous attempts [6]. Thus, one is perhaps forced to wonder if some other mechanism can solve the strong CP-problem. Presumably, any solution intrinsic to QCD will be nontrivial and nonperturbative [7, 8]. For example, Wu and Zee have analyzed the topology of the gauge orbit space, and speculated that θ is restricted to $\theta = 2\pi n$, $n \in \mathbb{Z}$, by an analogy with magnetic flux in a superconductor [9].

Another nonperturbative issue is the influence of θ on the dynamics of non-abelian gauge theories, in particular the confinement mechanism. There is numerical evidence that confinement at $\theta = 0$ is caused by the condensation of color magnetic monopoles [10]. In the θ-vacuum these monopoles acquire an electric charge $\theta/2\pi$; they become dyons [11]. This led 't Hooft to propose new "oblique" confinement phases, in which monopole–gluon bound states condense [12]. These phases are separated from the ordinary confined phase by phase transition(s) at some $\theta \leqslant \pi$. In an oblique confinement phase, a quark can bind to a dyon to form a liberated object with the flavor of the quark and the color magnetic charge of the monopole.

Finally, θ can be viewed as an artificial parameter which can be exploited to obtain information about the theory at $\theta = 0$. It is an imaginary chemical potential for the topological charge Q, so derivatives of the free energy with respect to θ measure the influence of topologically nontrivial configurations on the vacuum. Furthermore, these derivatives can be related to the mass and couplings of the η' meson [13].

With these ideas as motivation we have sought to analyze the θ-dependence of SU(N) gauge theory using numerical simulations of the lattice theory. A direct simulation of the θ-vacuum is impossible because the action has an imaginary part. However, one can generate configurations at $\theta = 0$ and include the Boltzmann factor $e^{-i\theta Q}$ in the measured observable. Large values of θ therefore require very large ensembles of gauge-field configurations for which Q has been evaluated, and this is the basic limitation of this approach. At present, sufficiently precise data have been published only for pure gauge (SU)2 [14], but, as we shall see, even it becomes inadequate once $\theta \approx \frac{1}{2}\pi$.

* Actually, in the standard model θ is replaced by $\bar{\theta} = \theta + \phi$, where ϕ is the phase of the determinant of the quark mass matrix; if any quarks are massless, one can choose ϕ so that $\bar{\theta}$ vanishes. We shall assume that none of the quarks is massless, and write θ for $\bar{\theta}$.

Several years ago a pilot investigation along these lines appeared [15]. However, this work was on a small lattice (5^4) at a small value of the gauge coupling ($\beta = 2.1$). Moreover, ref. [15] used a heuristic (though integer) prescription for the charge [16]. In contrast, we have lattices up to size 16^4, and a range of couplings $2.2 \leqslant \beta \leqslant 2.7$. Most importantly, we use the topological charge of Phillips and Stone [17], which is based on reconstructing a fiber bundle [18].

In sect. 2 we provide the basic formalism for discussing θ-physics. Sect. 3 contains the results of our analysis of the Monte Carlo data from ref. [14]. This includes the θ-dependence of the partition function, the free energy, and the "string tension", as well as the volume dependence of the η' self-coupling. We compare our results to the predictions of the dilute instanton gas [19]; for larger volumes, the numerical simulations deviate from this naive picture. Finally, sect. 4 provides some outlook.

2. θ-dependence of physical observables

We consider SU(2) lattice gauge fields U_ℓ with the Wilson action. In the θ-vacuum the expectation value of an operator is given by the path integral

$$\langle \mathcal{O} \rangle_\theta = \frac{\int [\mathrm{d}U_\ell] \mathcal{O}\, \mathrm{e}^{-S_\theta}}{\int [\mathrm{d}U_\ell] \mathrm{e}^{-S_\theta}}. \tag{2.1}$$

The functional integration over field configurations decomposes into a sum over sectors with common topological charge Q. The topological charge distribution (at $\theta = 0$) is

$$\mathsf{P}_Q = \frac{\int [\mathrm{d}U_\ell]_Q \mathrm{e}^{-S}}{\int [\mathrm{d}U_\ell] \mathrm{e}^{-S}}, \qquad \sum_Q \mathsf{P}_Q = 1, \tag{2.2}$$

where $[\mathrm{d}U_\ell]_Q$ denotes the functional measure on the charge-Q sector. The P_Q play a central role in our study of θ-effects because they are directly determined in the numerical simulations.

Observables which only depend on the topological charge can be obtained from the θ-dependent partition function

$$Z(\theta) = \sum_Q \mathsf{P}_Q \mathrm{e}^{-i\theta Q}, \tag{2.3}$$

and the associated "free energy" per spacetime volume V

$$F(\theta) = -\frac{1}{V} \ln Z(\theta). \tag{2.4}$$

Moreover, a phase transition in θ would be reflected by nonanalytic behavior of the partition function $Z(\theta)$ in the complex θ-plane. Actually, since numerical simulations necessarily work with infrared and ultraviolet cutoffs, we expect only an accumulation of zeros in $Z(\theta)$ [20].

The expectation value of some operator $\mathcal{O}[U_\ell]$ in the θ-vacuum can be written as a sum over different topological charge sectors

$$\langle\mathcal{O}\rangle_\theta = \frac{1}{Z(\theta)}\sum_Q \langle\mathcal{O}\rangle_Q \mathsf{P}_Q \mathrm{e}^{-i\theta Q}, \tag{2.5}$$

where

$$\langle\mathcal{O}\rangle_Q = \frac{\int [\mathrm{d}U_\ell]_Q \mathcal{O}\, \mathrm{e}^{-S}}{\int [\mathrm{d}U_\ell]_Q \mathrm{e}^{-S}} \tag{2.6}$$

denotes the expectation value of $\mathcal{O}$ in the sector with fixed topological charge Q. The connected moments of the topological charge distribution can be obtained directly from the free energy

$$\frac{1}{V}\langle Q^n\rangle_{\theta,\mathrm{c}} = -i^n \frac{\mathrm{d}^n F}{\mathrm{d}\theta^n}(\theta). \tag{2.7}$$

For example, the topological susceptibility, given by

$$\chi_\mathrm{t}(\theta) = \frac{\mathrm{d}^2 F}{\mathrm{d}\theta^2}(\theta) = \frac{1}{V}\left(\langle Q^2\rangle_\theta - \langle Q\rangle_\theta^2\right), \tag{2.8}$$

is especially interesting.

The simplest picture of the vacuum is the dilute instanton gas [19]. The topological charge distribution is obtained from a convolution of separate Poisson distributions for instantons and anti-instantons

$$\mathsf{P}_Q^{(ii)} = \sum_{n=0}^{\infty} \mathsf{P}_n^{(i)} \mathsf{P}_{Q-n}^{(i)}, \qquad \mathsf{P}_n^{(i)} = \mathsf{P}_{-n}^{(i)} = \frac{\langle Q^2\rangle_{0,\mathrm{c}}^n \exp\left(-\langle Q^2\rangle_{0,\mathrm{c}}/2\right)}{2^n n!}. \tag{2.9}$$

From eq. (2.9) one finds that the free energy of the dilute instanton gas is

$$F^{(ii)}(\theta) = \chi_\mathrm{t}(0)(1-\cos\theta), \tag{2.10}$$

which is regular in the complex θ-plane. Hence, this scenario has no phase transition in θ, contradicting oblique confinement.

At least in the large-N limit of SU(N), the topological susceptibility of the pure-glue theory at $\theta = 0$ is related to the mass of the η'-meson according to [13]

$$m_{\eta'}^2 = \frac{2N_\mathrm{F}}{f^2}\frac{\mathrm{d}^2 F}{\mathrm{d}\theta^2}(0)\bigg|_{\text{pure glue}}, \tag{2.11}$$

TABLE 1

Parameters of the simulations. The lattice size is always L^4, β is the gauge coupling, N_Q is the number of configurations for which the topological charge was computed, and "group" refers to the physical volume, as explained in the text.

L	β	N_Q	group	L	β	N_Q	group
6	2.3	5000	A	6	2.2	5500	B
8	2.4	12500	A	8	2.3	20000	B
8	2.5	3000	A	10	2.4	19069	B
10	2.5	7000	A	12	2.5	3200	B
12	2.6	2600	A				
12	2.7	1100	A				
16	2.7	1800	A				

where f is the large-N limit of the meson decay constant, and N_F is the number of light quark flavors. In the same context, the four-point η' self-coupling of the effective interaction vertex

$$V^{(4)}(\eta') = \frac{1}{4!} g_{\eta'}^{(4)} \eta'^4, \tag{2.12}$$

is determined by the fourth derivative of $F(\theta)$ [13]:

$$g_{\eta'}^{(4)} = -\frac{4N_F^2}{f^4} \frac{d^4F}{d\theta^4}(0)\bigg|_{\text{pure glue}} = \frac{2N_F}{f^2} m_{\eta'}^2 R, \tag{2.13}$$

where

$$R = \frac{\langle Q^4 \rangle_{0,c}}{\langle Q^2 \rangle_0}, \qquad \langle Q^4 \rangle_{0,c} = \langle Q^4 \rangle_0 - 3\langle Q^2 \rangle_0^2. \tag{2.14}$$

Even beyond the validity of eq. (2.13), R is an interesting quantity in the context of numerical simulations because it is universal, i.e. it is a dimensionless ratio of physical observables.

3. Analysis of the Monte Carlo data

In ref. [14] the probability distribution P_Q for a wide variety of lattices has been determined. The simulation parameters of the lattices included in the θ-vacuum analysis are listed in table 1. They fall into two groups. Group A corresponds to small to intermediate physical volumes with* $z_t = La\chi_t^{1/4} \leqslant 1.5$. In these volumes

* z_t is related to the conventional dimensionless measure of the physical volume, $z = L/\xi$, where ξ is the correlation length, by $z \approx 4.7 z_t$.

the spectrum is well described by a perturbative hamiltonian [21], and color magnetic monopoles are dilute [10], indicating that confinement has not yet set in dynamically. Also, the dilute instanton gas becomes a reliable approximation [22]. Group B corresponds to larger physical volumes, $z_t \geqslant 1.5$; here the validity of the perturbative hamiltonian breaks down, and the monopoles condense – the dynamics of confinement emerge. One also can no longer assume that the dilute instanton gas picture is valid; long-range correlations might induce significant interactions between the topological charge carriers.

Fig. 1 displays the charge distributions obtained on ensemble $\mathscr{A}$, $L=8$ at $\beta=2.4$, from group A, and on ensemble $\mathscr{B}$, $L=10$ at $\beta=2.4$, from group B. The two distributions are somewhat different in the region of small charges. Ensemble $\mathscr{B}$'s distribution is flatter, and its fluctuations are greater. Since the partition function is the Fourier transform of P_Q, we anticipate an effect for larger values of θ. The partition function $Z(\theta)$ for these two ensembles is shown in fig. 2, together with the dilute gas prediction using the susceptibility determined in the simulation. In the small volume, fig. 2a, we find agreement with the dilute gas, within the errors. This was seen also in ref. [15], which also had $z_t < 1.5$. On the other hand, in the larger volume, fig. 2b, we observe a zero in $Z(\theta)$ around $\theta/\pi = 0.35$ – this result is perhaps a first indication of the accumulation of zeroes that signals a phase transition [20]. The partition function determined from the numerical simulations has too few zeroes in the complex plane to see any accumulation, because in practice we have the P_Q only for a restricted range of Q. The deviation of $Z(\theta)$ from the dilute gas is a 2–3 standard error effect. Throughout, we determine the errors after binning the data into subensembles, and the statistical significance is stable against different binning procedures. For θ-dependent quantities the solid line indicates the central value, and the dashed lines a one standard error fluctuation.

Fig. 3 shows the normalized free energy, $F(\theta)/\chi_t(0)$, for all lattices in the two groups, again compared to the dilute-gas prediction. The dashed error curves are omitted for clarity. For small volumes, fig. 3a, we find agreement up to $\theta/\pi \approx 0.55$, beyond which the statistical errors become too large to draw any conclusions. For the larger volume, fig. 3b, the free energy diverges at the zero of the partition function; note that all group B lattices have a zero in the range $0.30 \lesssim \theta/\pi \lesssim 0.40$.

The θ-dependence of the normalized topological susceptibility, $\chi_t(\theta)/\chi_t(0)$, is shown in fig. 4. In this case statistical uncertainties are tolerable only in a small range of θ, in which both groups agree with dilute-gas behavior (within errors). Note, however, that even the central value from ensemble $\mathscr{A}$ is consistent with the dilute gas, whereas the central value from ensemble $\mathscr{B}$ is not.

Besides purely topological quantities, we have studied the θ-dependence of the energy of a unit of 't Hooft electric flux, E_0; in the string picture of the vacuum $E_0 = LaK$, for large L, where K is the string tension. We extract aE_0 from the exponential decay of the correlation function of Polyakov loops, $\Sigma_{x_\perp} \langle P(x_\perp, t) P(0_\perp, 0)\rangle_\theta$. For each value of θ we fit the correlation function to a

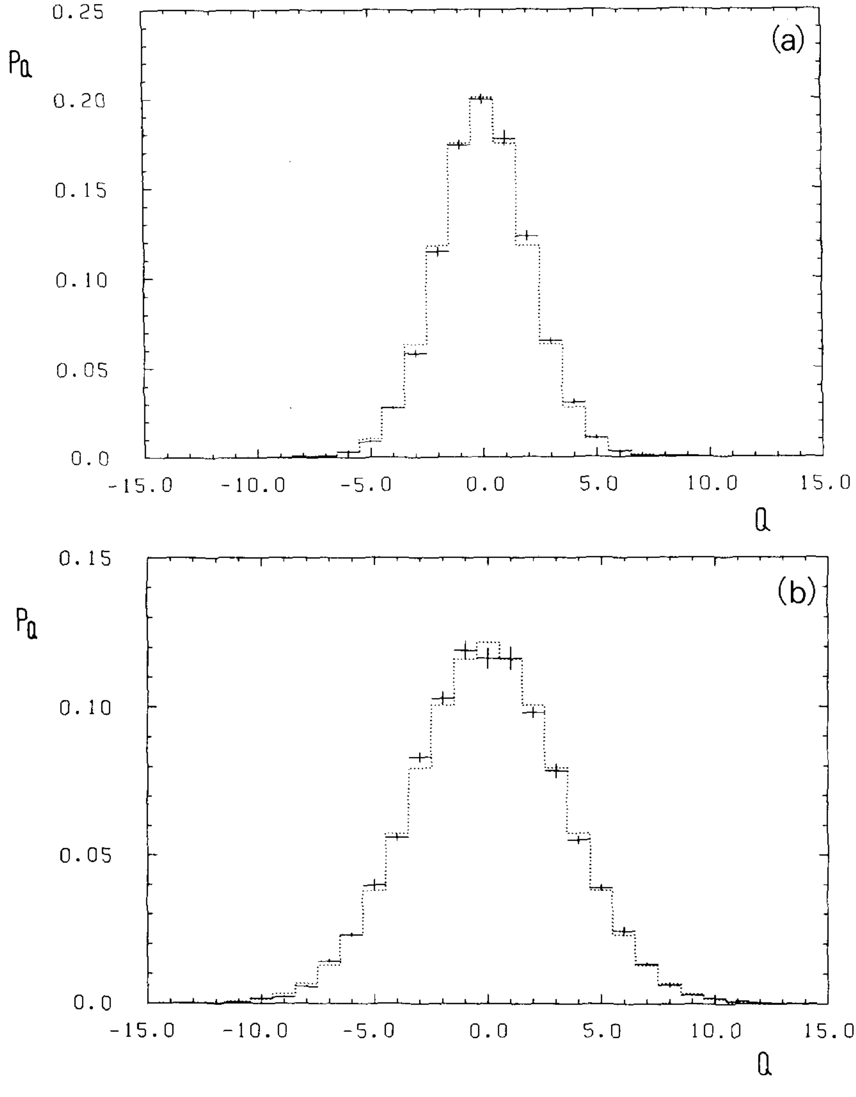

Fig. 1. Charge distributions of: (a) ensemble $\mathscr{A}$ at $L=8$, $\beta=2.4$, typical of group A; and (b) ensemble $\mathscr{B}$ at $L=10$, $\beta=2.4$, typical of group B. The dotted histograms indicate the dilute gas prediction, whereas the solid lines with error bars indicate the Monte Carlo simulations.

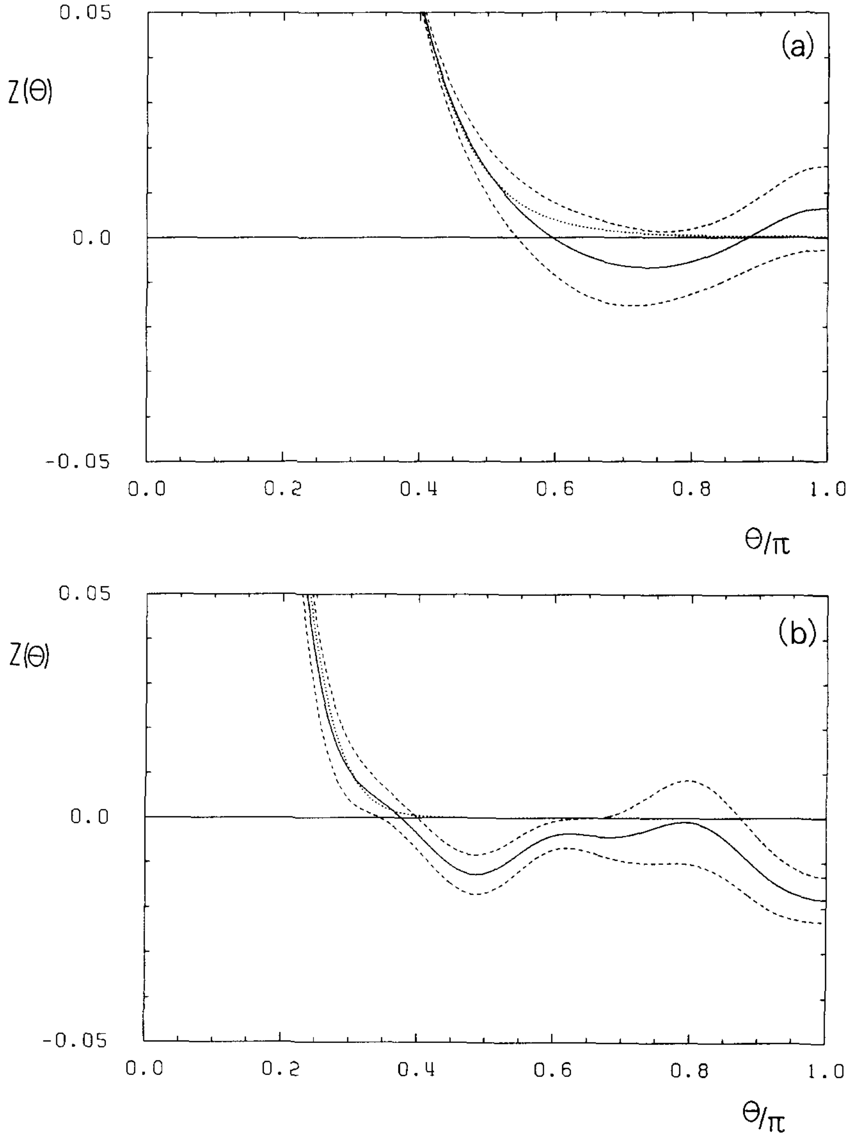

Fig. 2. Partition function $Z(\theta)$ as a function of θ for (a) ensemble $\mathscr{A}$, (b) ensemble $\mathscr{B}$. The dashed line indicate a one standard error fluctuation, and the dotted lines indicate the dilute gas prediction.

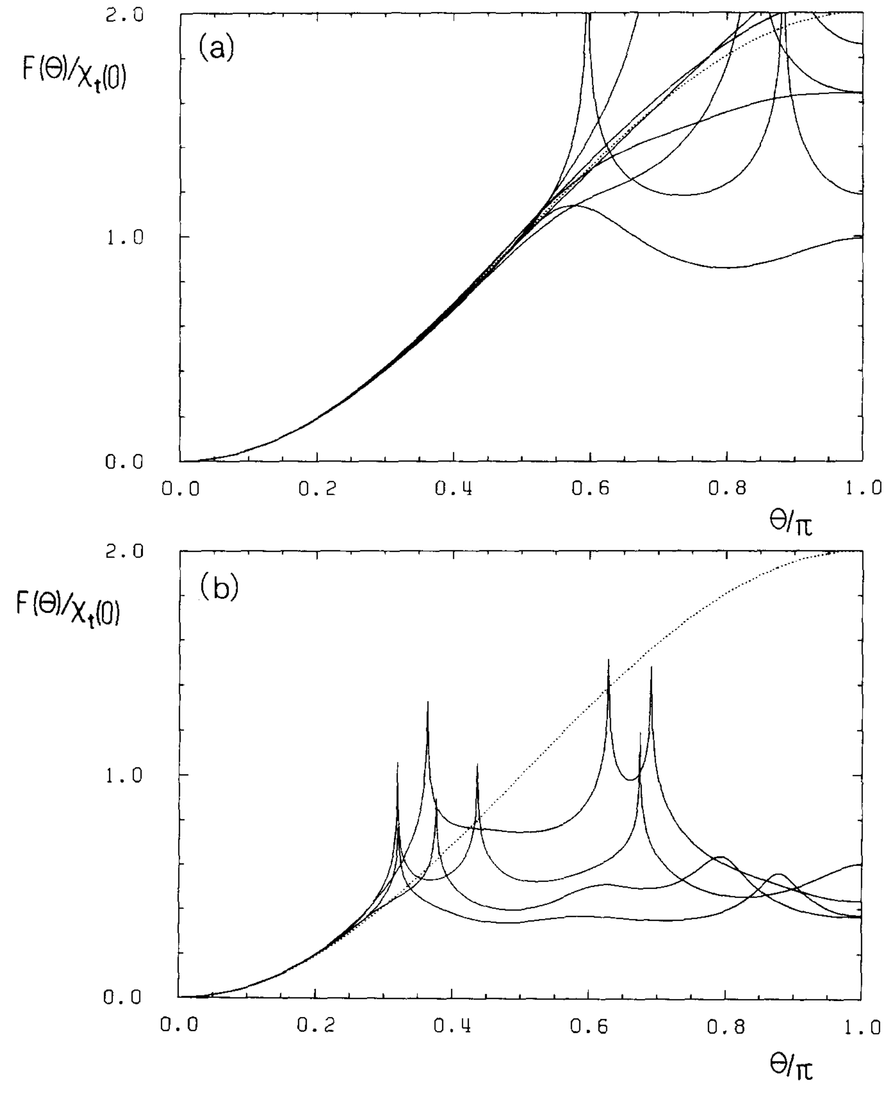

Fig. 3. Free-energy density (normalized by the susceptibility) $F(\theta)/\chi_t(0)$ as a function of θ, for (a) all of group A, (b) all of group B. The dotted lines indicate the dilute gas prediction.

single hyperbolic cosine, discarding the first two timeslices. The results for the $L = 12$, $\beta = 2.5$ ensemble and ensemble $\mathscr{B}$ are shown in fig. 5. It turns out that $E_0(\theta)$ does not vary much for $\theta/\pi \lesssim 0.2$, indicating that color is still confined in this range. At larger values of θ the statistical fluctuations become overwhelming. We should mention, however, that on these lattices finite-volume effects and scaling violations of the electric flux energy are sizeable. We also cannot rule out the

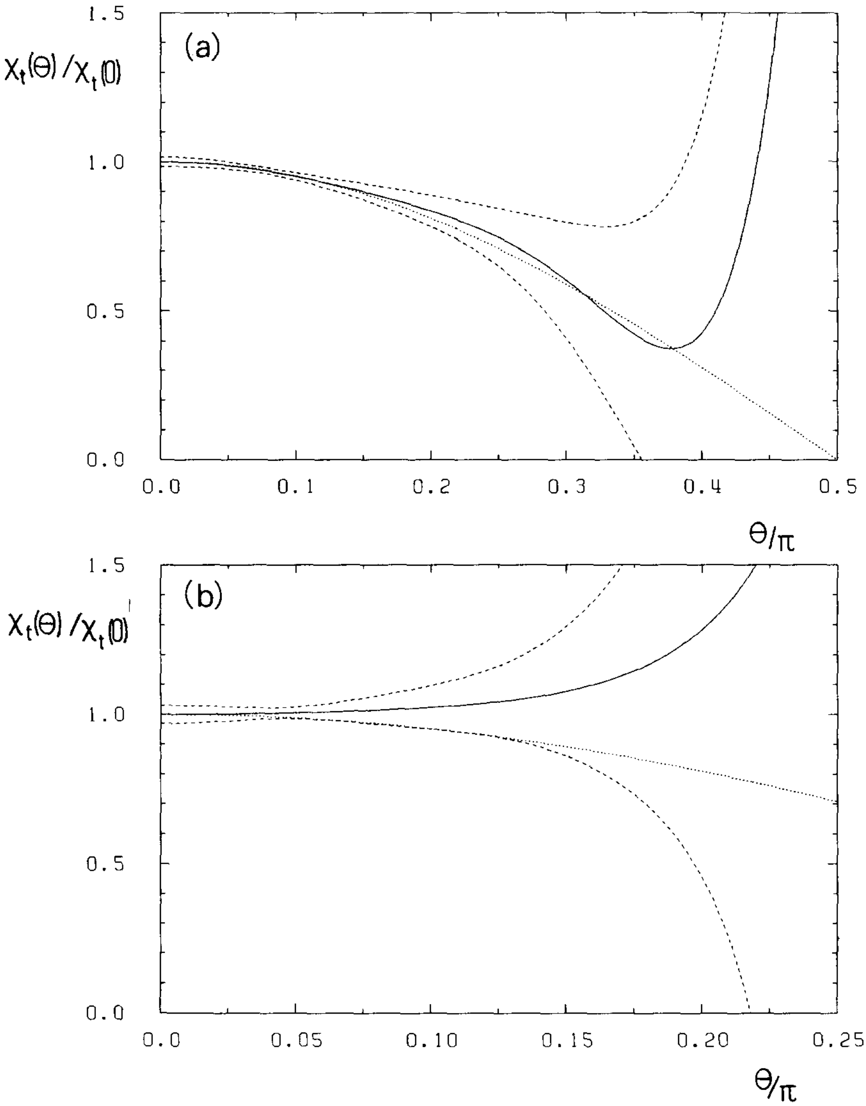

Fig. 4. Normalized topological susceptibility $\chi_t(\theta)/\chi_t(0)$ as a function of θ for (a) ensemble $\mathscr{A}$ (b) ensemble $\mathscr{B}$. Note that the horizontal scales differ, and that both differ also from the previous figures The dashed lines indicate one standard error fluctuations, and the dotted lines indicate the dilute gas prediction.

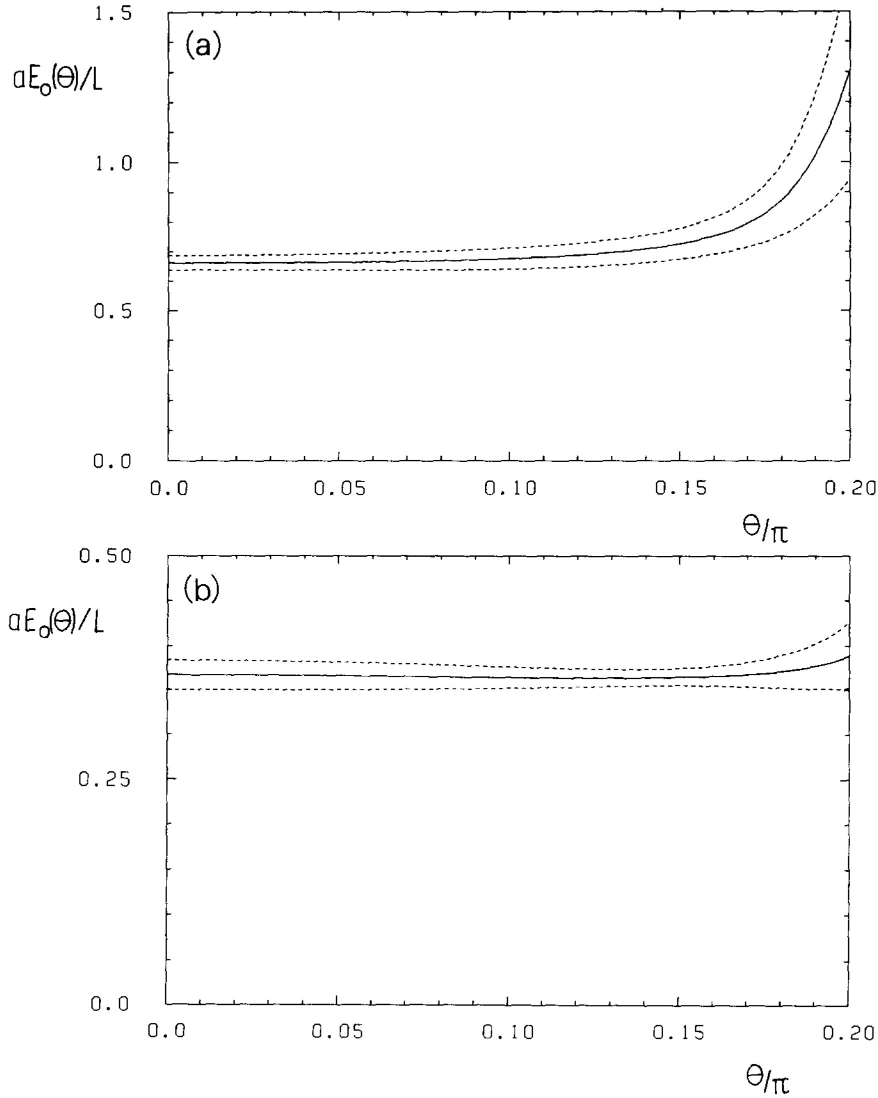

Fig. 5. "String tension" aE_0/L obtained from the 't Hooft electric flux as a function of θ for (a) the $L=12$, $\beta=2.5$ ensemble, (b) ensemble $\mathscr{B}$. The dashed lines indicate one standard error fluctuations.

possibility that lattice artefacts – the dislocations – wash out the θ-dependence of E_0 even in this β range [23].

The z_t dependence of the quantity R, defined in eq. (2.14), is plotted in fig. 6, including also some other simulations from ref. [14]. In particular, the solid points come from simulations from the mixed fundamental–adjoint action, so that fig. 6 also shows a test of universality. In the dilute gas picture, one has $R=1$, which the

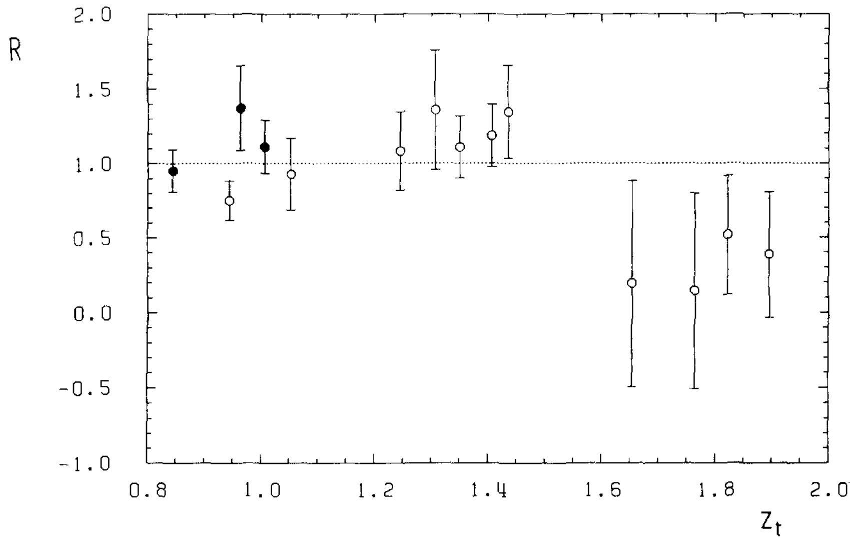

Fig. 6. The ratio R of eq. (2.14) as a function of z_t; all simulations from both groups are included, as well as a few more from ref. [14]. The solid points were obtained using the mixed fundamental–adjoint action. The dilute gas predicts $R = 1$.

small-volume simulations substantiate. However, at $z_t \approx 1.5$ the ratio R drops rapidly to $R \approx 0.3$. Through eq. (2.13) it implies an η' self-coupling [13] which is rather weaker than in the dilute gas model. In fact, R is also consistent with zero, for $z_t \gtrsim 1.5$, which perhaps indicates that the free energy is of the form $F(\theta) \propto \theta^2$, as conjectured by Affleck [24]. The conjecture is supported by the third moment $\langle Q^3 \rangle_{\theta, c}$, which is consistent with zero, for $z_t \gtrsim 1.5$.

4. Conclusions

Calculations of the spectrum [21, 25–27], the topological susceptibility [14, 22], and the density of color magnetic monopoles [10] point to a coherent picture of QCD in finite volumes. In small volumes the physics is well described by perturbative and/or semiclassical techniques. However, around $z_t \approx 1.5$ ($z = L/\xi \approx 7$, $\xi =$ correlation length) a qualitative change takes place, and the vacuum becomes truly nonperturbative. Our analysis of the θ-vacuum in SU(2) lattice gauge theory supports this picture. For simulations with $z_t < 1.5$ we found no significant deviation from a dilute instanton gas. On the other hand, for $z_t > 1.5$ we found some surprises: most remarkable are the zero in $Z(\theta)$ at $\theta \approx 0.35\pi$ and the rapid drop in R. These intriguing results deserve to be strengthened by more simulations. Unfortunately, one would need about 100 times better statistics to attain precise enough charge distributions.

There is little we can say about the strong *CP*-problem. In the Wu–Zee [9] scenario, the free energy $F(\theta)$ has a deep well at $\theta = 2\pi n$. The physical picture is that the dynamics might tune θ to minimize $F(\theta)$. To realize this, QCD probably needs to be coupled to some other system, which would carry off the energy. At an early stage of our runs the large-z_t Monte Carlo data appeared to support the Wu–Zee free energy. However, the higher statistics analyzed here do not really encourage any speculation.

In order to test the ideas of refs. [9,12] and others, the Monte Carlo methods must be refined. This might be possible using the techniques of refs. [28] to compute simultaneously the β *and* θ dependence of the partition function. The variation for complex actions proposed by Gocksch [29] appears especially promising, and we are now testing it. Applied to the θ-vacuum, this would mean running Monte Carlo simulations at fixed Q, keeping a record of how eager the simulation is to leave the fixed-charge sector. This technique would allow us to determine P_Q for very large values of Q, which do not appear in conventional Monte Carlo runs. With a large range of Q the numerical approximation to $Z(\theta)$ will have more zeros, and the hypothesis of a phase transition [12] could be tested. Whether even more esoteric speculations can be tested, like those touching the strong *CP*-problem [9], remains to be seen.

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