Topological Charge in Lattice Gauge Theory

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(Received 9 May 1983)

A useful definition of the topological charge of a lattice gauge-field configuration is given. This definition is used to calculate the topological susceptibility $\chi_t = \langle Q^2 \rangle / V$ in SU(2) lattice gauge theory by means of a Monte Carlo simulation. $\chi_t = (170 \pm 25 \text{ MeV})^4$ is obtained, in good agreement with the current algebra prediction. Other possible uses of this operator are suggested.

PACS numbers: 11.15.Ha

Non-Abelian SU(N) gauge-field configurations on a compact four-dimensional space can be classified topologically by an integer Q, given by¹

 $Q = (g^2/32\pi^2) \int d^4x \operatorname{Tr}[F\tilde{F}(x)].$

The physical consequences of this are of some interest; they include the resolution of the U(1) problem, the existence of θ vacua, and a possible mechanism for chiral symmetry breaking.² In this paper I will suggest a definition of the topological charge Q in the context of lattice gauge theory,³ and use it to compute the topological susceptibility $\chi_t = \langle Q^2 \rangle / V$ in the SU(2) lattice gauge theory.

Witten has shown,⁴ using large-*N*-approximation arguments, that this quantity is related to the mass of the η' . An extended current algebra using these ideas has been developed, in which the relation

$$\chi_t = (f_{\pi^2}/2N_f)(m_{\eta^2} + m_{\eta'}^2 - 2m_k^2) = (180 \text{ MeV})^4$$

can be derived.⁵ Calculation of this quantity in lattice gauge theory was first attempted in Ref. 6, with use of a definition of Q which is unsatisfactory, since it is not a total divergence and thus does not give a topological invariant. Berg and Lüscher⁷ have given a definition of Q for the nonlinear σ model which is geometrically more satisfactory, but the gauge-theory case is considerably more subtle.

I will first give a heuristic discussion of the way in which topological nontriviality arises in continuum gauge field theory, as a preliminary step in dealing with the lattice case. Gauge-invariant quantities such as Wilson loops are physically observable and in an asymptotically free theory such as QCD we expect these quantities to be nonsingular at the scale of the cutoff throughout space-time except at the positions of charged particles or monopoles. The vector potential, which is what appears in the functional integral quantization, has no physical reason to be nonsingular, and so we must integrate over singular as well as nonsingular vector potentials. A gaugefield configuration that is given by a nonsingular vector potential everywhere on a compact manifold M will be topologically trivial, since $\operatorname{Tr}[F\tilde{F}(x)]$ is a total derivative.

The topological significance of the gauge-dependent singularities in the vector potential can be seen as follows: Consider a neighborhood Ncontaining a point where the vector potential is singular. Now make a gauge transformation $\Phi(x)$ on the fields in **N** that removes the singularity. Our initial singular field configuration on M is now described by a field configuration that is nonsingular, but is in different gauges in N and in the rest of *M*. The description of the configuration is completed by giving the transition function on ∂N which tells how to transform between the two different gauges. This transition function gives a nonsingular mapping from ∂N into the group G and now carries all the information about the topology of the configuration. For an n-dimensional manifold M, ∂N is topologically an (n-1)-sphere S^{n-1} . The maps $S^{n-1} \rightarrow G$ are topologically classified by the homotopy groups $\pi_{n-1}(G)$. In the case of interest to us, the relevant homotopy group is $\pi_3(SU(N)) = Z$, and so our configurations will be classified by an integer. Thus, to determine the topological charge of a gauge field configuration we must locate the gauge singularities, locally gauge transform them away using different gauges, and measure the degrees of the maps relating the different gauges. The sum of these degrees will be a topological invariant, the topological charge.

A lattice gauge-field configuration is given by a set of group elements, $U_{\mu}(n)$, one for each link connecting neighboring sites on the lattice. When considering the question of what topological significance can be assigned to a lattice gauge-field configuration, one is tempted to conclude that lattice gauge fields cannot be assigned a definite topological charge, since the limited amount of information about the corresponding continuum configuration that is coded in the link variables is not enough to fix the topology. Different interpolations constructed from the given information about the vector potential on the links would give different topological charges. In particular, it seems that we should be able to view the lattice configuration as corresponding to a smooth continuum configuration, and this would always be topologically trivial.

In the case of a lattice theory near the continuum limit, the coupling g(a) is small so that the fluctuations in the Wilson loops at the scale of a lattice spacing are small and there are no fluctuations on scales smaller than a lattice spacing. The constraint that the Wilson loops be near the identity at and below the scale of a lattice spacing is what allows us to assign a topological charge to a lattice field configuration. A smooth interpolation of the vector potential between the lattice links may introduce values for some small Wilson loops which are far from the identity in the group. In order to avoid this we are forced into the introduction of singular interpolating vector potentials.

The above considerations lead us to a natural definition of the topological charge in the fourdimensional case. For each hypercube in the lattice, interpolate the gauge fields from the links throughout the hypercube in such a way as to keep all Wilson loops near the identity. This will always be possible if the plaquette variables of the original configuration are close to the identity. Now gauge transform this interpolated configuration to a gauge where the vector potential is small everywhere. The contribution of the hypercube to the topological charge will be just the degree of this gauge transformation on the boundary of the hypercube.

This definition is geometrically straightforward but, like the one proposed by Lüscher,⁸ complicated and time consuming to carry out in practice, since the gauge function must be constructed on a rather fine grid on the boundary of each hypercube. A more tractable method for computing the topological charge will now be described, based on the idea of defining different gauges in regions of the lattice larger than a single hypercube, in order to express the topological charge in terms of the degrees of more wellbehaved mappings. This method is only one of a general class of similar methods and, while it does not properly reconstruct the topological charge for all configurations, it seems to be satisfactory for measuring the topological susceptibility in the scaling region $\beta = 2.2$ to 2.4.

The basic idea is that if one locally makes links small by means of a gauge transformation $\Phi(x)$, Φ will not be a smooth mapping, but

$$\theta_{ii'}(x) = \Phi_i(x) \Phi_{i'}^{-1}(x),$$

the transition function between two neighboring coordinate patches indexed by i and i', will tend to be smooth. Thus we would like to reexpress the topological charge in terms of these quantities.

The lattice is broken up into "time slices" T_i , defined by

$$T_i = \{ (\mathbf{x}, t) \in M = T^4; \quad i \leq t \leq i+1 \}$$

which overlap along a constant-time three-torus. The topological charge in this situation will be

$$Q = \sum \text{degree}[\theta_{i,i+1}(x)].$$

The prescription that I have used for determining the gauge within each T_i is the following: Choose $\Phi_i(x)$ in T_i such that (a) the spacelike gaugetransformed links at t = i, $U_{\mu'}(n)$, satisfy

$$\sigma = \sum_{n,\mu} (1 - \mathrm{Tr} U_{\mu}')$$
 is a minimum;

(b) $U_0'(n) = 1$. Condition (a) is implemented iteratively starting with some random $\Phi_i(x)$, and stepping through the lattice, choosing a new $\Phi_i(x)$ at each site in such a way as to minimize σ .

Now that $\Phi_i(x)$ has been determined at t = i, condition (b) is implemented by the choice

$$\Phi_i(\mathbf{x}, i+1) = \Phi_i(\mathbf{x}, i) U_0(\mathbf{x}, i).$$

 $\Phi_i(\mathbf{x})$ is now defined at each lattice site and the $\theta_{i,i+1}$ are determined by

$$\theta_{i,i+1}(x,t=i+1) = \Phi_i(x,t=i+1)\Phi_{i+1}^{-1}(x,t=i+1)$$

With a little thought one can see that if the gaugetransformed link between \mathbf{x} and $\mathbf{x} + \mu$ is near the identity at t = i and t = i + 1, and the plaquette angle for the timelike plaquette involving these two links is also small, then the angle between the $\theta_{i,i+1}$ at the neighboring sites that share the link will again be small. In this case the degree of the mapping defined by $\theta_{i,i+1}$ can be unambiguously determined.

The weak point of this definition is that, in general, it may not be true that all the gauge-transformed spacelike links are sufficiently close to the identity to define the transition function unambiguously. However, the numerical evidence from use of this algorithm in the scaling region is that typically all but a very small number of links will be close to the identity, and that those that are not do not often conspire to produce an incorrect value for the topological charge.

The degree of a continuous mapping from some three-dimensional compact space into S^3 is just the number of times S^3 is swept out by the mapping. Equivalently, the degree is the volume swept out by the mapping divided by the total volume of the three sphere. If the $\theta_{i,i+1}$ at neighboring sites are close together in S^3 , there is an obvious notion of the volume swept out by $\theta_{i,i+1}$.

The $\theta_{i,i+1}$ are defined at the sites given by a cubical decomposition of the three-torus consisting of the lattice at constant time t = i. Each of these cubes can be decomposed into six tetrahedra. Each such tetrahedron is mapped by θ into a spherical tetrahedron in S^3 . Except for a set of degenerate configurations of measure zero involving large angles between neighboring $\theta_{i,i+1}$, the volume of such a spherical tetrahedron is uniquely defined. Summation over the volumes of these tetrahedra will give an integer times the volume of S^3 ; this integer is the degree.

It turns out that there is a simple trick which can be used to compute the degree when the value of the contribution from each individual tetrahedron is not needed. Pick an arbitrary point on S^3 , and for each of the tetrahedra in S^3 decide whether the point is inside or outside the tetrahedron. If it is inside, add +1 to the expression for the degree if the mapping preserves the orientation of the tetrahedron, -1 if it reverses the orientation. This sum over all the tetrahedra will give the same answer for the degree as the sum over all the volumes, but it is much easier to calculate numerically, involving only the calculation of a



FIG. 1. Topological susceptibility for SU(2) lattice gauge theory on a 6^4 lattice.

few small determinants for each tetrahedron.

A Monte Carlo calculation of $\langle Q^2 \rangle / V$ was performed for SU(2) lattice gauge theory on a 6⁴ lattice, using a program based on that of Bhanot, Lang, and Rebbi.⁹ The results are plotted in Fig. 1. Each datum point in the scaling region corresponds to 300 measurements of the topological charge on configurations derived from six different runs beginning with different initial configurations.

Renormalization-group arguments demand that the lattice spacing vary with the coupling as

$$a(\beta) = \left(\frac{6\pi^2}{11}\beta\right)^{51/121} \exp\left(-\frac{3\pi^2}{11}\beta\right).$$

Thus we expect χ_t to scale as

$$\chi_{t} = \frac{\langle Q^{2} \rangle}{V} = \frac{\langle Q^{2} \rangle}{N^{4} a^{4}}$$
$$= \frac{\langle Q^{2} \rangle}{N^{4}} \Lambda_{L}^{4} \left(\frac{6\pi^{2}}{11}\beta\right)^{-204/121} \exp\left(\frac{12\pi^{2}}{11}\beta\right).$$

The Monte Carlo data for $\langle Q^2 \rangle / N^4$ behave exactly as predicted, giving

 $\chi_t = [(31.5 \pm 2.5)\Lambda_L]^4 = [(1.59 \pm 0.11)\Lambda_{\overline{MS}}]^4$

(using Ref. 10), which implies

 $\Lambda_{\overline{MS}} = 113 \pm 8$ MeV.

Comparison with Creutz's result¹¹ for the string tension gives

$$\chi_t = [(0.4 \pm 0.06)\sqrt{\sigma}]^4$$

and, use of

 $\sqrt{\sigma} = 420 \text{ MeV}$

gives

$$\chi_t = (170 \pm 25 \text{ MeV})^4$$
,

consistent with the experimental value.

One expects to observe a suppression of the topological charge at large β for small lattices; that this is not observed indicates that the method used here for measuring the topological charge is not entirely satisfactory. If the algorithm misidentifies the topological charge a small fraction of the time, this will make little difference until β is greater than around 2.4, where, since the real topological charge is essentially always zero, the small fraction of errors becomes the dominant contribution to $\langle Q^2 \rangle$. In a future paper, I will report on an improved algorithm which deals with this problem, but I believe that this is irrelevant to the result for the topological susceptibility. Note that at $\beta = 2.5$, where presumably all topological charge has been suppressed by the finite size of the lattice, the algorithm gives Q = 0 90% of the time, which perhaps gives some idea of the error rate in the scaling region.

There are quite a few other interesting calculations that are made possible by this work, including the following:

(i) Extension of the calculation to the case of SU(3).

(ii) Use of this method to check the reliability of semiclassical approximations, including the picture of the QCD developed by Callan, Dashen, and Gross.¹²

(iii) Calculation of θ vacuum expectation values for various operators. One could try to determine the phase structure of QCD as a function of θ , and see if the picture of "oblique confinement" is realized as suggested by 't Hooft.¹³

(iv) Measurement of the topological charge in fermion Monte Carlo calculations. This could lead to a better understanding of the role played by fermion zero modes in chiral-symmetry breaking.

I would like to thank my thesis advisor Curtis G. Callan, Jr., who suggested this project, and

C. Whitmer for his help with the computer program. This work was supported in part by the National Science Foundation Grant No. PHY-80-19754.

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