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Positivity and topology in lattice gauge theory

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The admissibility condition usually used to define the topological charge in lattice gauge theory is incompatible with a positive transfer matrix.

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With certain smoothness assumptions, continuum Yang-Mills field configurations in four dimensional spacetime can be classified by a topological winding number [1]. This realization has played a major role in our understanding of the importance of nonperturbative phenomena in the SU(3) gauge theory of the strong interactions [2].

This winding number is uniquely defined for smooth fields; however, for a quantum field theory one must integrate over all configurations, some of which may not be sufficiently smooth for a unique definition of the topological charge. Regulating the theory on a lattice brings in questions of how to handle these topological objects as their size drops below the lattice spacing. Considerable recent progress in this area has involved the use of Dirac operators with exact symmetries under chiral transformations [3–5]. Indeed, a rigorous lattice extension of the continuum index theorem relates the winding number to the zero eigenvalues of these chiral operators.

Classifying fields by their winding number divides the space of configurations into distinct topological sectors. With conventional actions, however, the configuration space is simply connected. Thus the winding number must be singular as one moves from one sector to another [6]. The locations of these singularities will in general depend on the particular Dirac operator used to define the topology. This ambiguity can be avoided by placing a constraint on the roughness of the gauge fields [7–9]. As usually formulated, the constraint forbids plaquettes to stray further from the identity than a given distance.

At first sight this constraint seems quite harmless, and, indeed, it is irrelevant to all perturbative physics. However, in this paper I show that such a constraint is incompatible with requiring a positive transfer matrix [10–12]. The argument builds on an old discussion of Grosse and Kuhnelt [13] that shows the failure of positivity for the Manton action [14].

I work with the gauge fields alone, and restrict myself to single plaquette actions. In the path integral, I assume the action associates a real non-negative weight $W(P)$ to any given plaquette, where the plaquette variable P is in the gauge group. I assume that $W(P)$ is smooth, indeed analytic, for P in some small vicinity of the identity. This insures a smooth mapping onto the perturbative limit. Away from the identity, I only assume it is piecewise smooth. The admissibility condition states that $W(P)$ should vanish for P in a finite region of the group some distance away from the identity.

To show that such a condition conflicts with positivity, I start by paralleling the argument of Ref. [13] and reduce the issue to a single timelike plaquette. If positivity holds, the matrix element of the transfer matrix between arbitrary states must be non-negative. In particular, for any square integrable function $\psi(g)$ over the group, one must have

$$\int dg' dg \psi^*(g') W(g'^{-1} g) \psi(g) \geq 0. \quad (1)$$

As a violation of this for any subgroup would imply a violation for the full group, I restrict the discussion to a U(1) subgroup. Denote the elements of this subgroup as $e^{i\theta}$, with $\theta = 0$ representing the identity element. I then should have

$$\int_{-\pi}^{\pi} d\theta' d\theta \psi^*(\theta') W(e^{i(\theta-\theta')}) \psi(\theta) \geq 0, \quad (2)$$

for arbitrary square integrable $\psi(\theta)$. Note that the restriction to a U(1) subgroup does not place any serious constraint on the allowed values of the plaquette. For example, in SU(3) the eighth Gell-Mann matrix generates a subgroup where $\frac{1}{3}\mathrm{ReTr}g$ runs over the full allowed region from $-\frac{1}{2}$ to 1.

Reduced to a U(1) subgroup, it becomes convenient to work with the Fourier functions $\psi(\theta) = e^{in\theta}$. Inserting one of these into the above and changing variables to $\phi = \theta - \theta'$ gives

$$f_n \equiv \int d\phi W(e^{i\phi}) e^{in\phi} \geq 0. \quad (3)$$

Thus all Fourier components of W must be real and non-negative, an extremely strong constraint. As is well known, any piecewise smooth weight can be reconstructed from its Fourier components

$$W(e^{i\phi}) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} f_n e^{-in\phi}. \quad (4)$$

Reality of the weight gives $f_{-n} = f_n$.

I now extend W into the complex plane. For this I define $z = e^{-i\phi}$, so that the physical weight function occurs on the unit circle. Separating the positive and negative terms in the series with the definition

$$f_+(z) = \sum_{n=1}^{\infty} f_n z^n, \tag{5}$$

I write

$$W(z) = f_0 + f_+(z) + f_+(1/z). \tag{6}$$

The assumption that the weight is analytic near $z = 1$ coupled with the positive nature of the f_n implies that one can also expand $f_+(z)$ about the origin with a radius of convergence z_0 greater than unity. Thus, the function $f_+(z)$ is analytic inside a circle of this radius about the origin. For the remaining piece contained in $f_+(1/z)$, I instead have an analytic function of z outside a circle of radius $1/z_0 < 1$. Thus the full weight $W(z)$ must be an analytic function in the common region, i.e., a ring with $1/z_0 < |z| < z_0$.

This analyticity immediately precludes many possible actions. For the present case, if $W(z)$ vanishes on any finite region of the unit circle, it must vanish everywhere, contradicting using it as a weight in a path integral. This is the main result of this paper.

Note that the weight can vanish at a finite number of discrete points. For example, $W = 1 + \cos(\theta)$ satisfies the positivity condition while being zero at $\theta = \pi$. It is only vanishing over a continuous region that is forbidden. The above proof also gives an explicit procedure for finding a wave function for which the transfer matrix is ill behaved; just calculate the Fourier coefficients successively until you find one that is not positive.

The positivity of the Fourier coefficients is a special case of the requirement that in a character expansion of $W(P)$ all coefficients must be positive [15]. This follows from using representation matrix elements for the wave functions in Eq. (1). This shows that the character expansion is absolutely convergent, and the analyticity extends to the entire group. Except for possible isolated points, there must be a finite probability of reaching any plaquette value.

So far the admissibility condition is the only way proven to give a uniquely defined topological index. However, this does not necessarily preclude the existence of some other smoothness condition to accomplish the same. The generality of the present result shows that any such condition cannot be a local constraint depending only on individual plaquettes.

Of course, positivity may not be a necessary requirement if the nonpositive effects disappear in the continuum limit. Indeed, such possibilities have been discussed in the context of generalized gauge actions, e.g., Refs. [16,17]. But it seems a large price to pay just to define an esoteric object such as the topological susceptibility.

As for the existence of the continuum Yang-Mills theory, it does not appear that a nonperturbative ambiguity in the definition of the topological susceptibility causes any harm. This concept is rather abstract, and it is not clear if it can be measured in any physical experiment, even considering external sources.

With several species of degenerate quarks, there is one point where the topological susceptibility is well defined. This is the chiral point, where the existence of massless Goldstone bosons uniquely fixes the quark masses to zero. Using a Ginsparg-Wilson formulation for the fermions then ensures that the topological susceptibility vanishes.

For one flavor of massless quark, the issue is less clear. Reference [18] argues that in the one quark case, the massless quark theory may have a scheme dependent continuum limit. If so, the point of vanishing topological susceptibility is also ambiguous.

Going to the pure glue theory, i.e., $n_f = 0$, the absence of a fermion determinant will allow the gauge fields to become even rougher. Recent discussions [19,20] of measuring the topological susceptibility with an external Ginsparg-Wilson operator have shown that all perturbative divergences are controlled. However, nonperturbatively, different operators have the potential to give different answers for the susceptibility for the same physical continuum limit. This is ruled out if the admissibility condition is satisfied, a condition inconsistent with positivity in the regulated theory.

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