Instantons and the Chiral Phase Transition

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Abstract

We examine the role of instantons in the zero-temperature chiral phase transition in an $SU(N)$ gauge theory. For a range of $N_f$ (the number of fermion flavors) depending on $N$, the theory exhibits an infrared fixed point at coupling $\alpha_*$. As $N_f$ decreases, $\alpha_*$ increases, and it eventually exceeds a critical value sufficient to trigger chiral symmetry breaking. For the case $N = 2$, we estimate the critical values of $N_f$ and $\alpha_*$ due to instantons by numerically solving a gap equation with an instanton-generated kernel. We find instanton effects of strength comparable to that of gluon exchange.

Instanton configurations $[1]$ of the Yang-Mills potentials $A_\mu(x)$ have been studied extensively for over two decades. They play a central role in the solution of the QCD $U(1)$ problem $[2]$, and a host of other physical consequences have been examined $[3]$. In particular, many authors have studied their possible role in the dynamical breaking of chiral symmetry in QCD $[4, 5, 6, 7, 8]$. All these studies face a difficulty: their effects are dominated by large instantons, on the order of the inverse confinement scale of the theory, where the interactions become strong and instantons overlap. Reliable quantitative estimates are therefore difficult.

A recent paper $[9]$ suggested that the chiral phase transition in an $SU(N)$ theory at zero temperature, as a function of the number of fermions $N_f$, could be analyzed without the complications of confinement. For a certain range of $N_f$, the two-loop $\beta$ function has an infrared stable fixed point, with the fixed point coupling $\alpha_*$ increasing as $N_f$ decreases. The transition was argued to set in when $\alpha_*$ exceeded a certain critical value. That work considered forces arising solely from gluon exchange.

Here, we examine the role of instantons in the same theory. The fixed point allows a more reliable study of instanton effects because it limits the growth of the effective
coupling at the large length scales which dominate the dynamics, better controlling the integration over the size of single instantons. We will begin our presentation with a brief review of the model; then display a gap equation with a kernel appropriate to an instanton background; next qualitatively consider the nature of possible solutions before displaying numerical results; and finally discuss reliability and draw some physical conclusions.

We write the Lagrangian for $SU(N)$ gauge theory as

$$\mathcal{L} = \bar{\psi}(i \partial - g A^a T^a)\psi - \frac{1}{4} F_{\mu\nu}^a F^{a\mu\nu} + \text{(gauge fixing terms)},$$

where $g$ is the gauge coupling, $\psi$ describes $N_f$ flavors of Dirac fermions in the $SU(N)$ fundamental representation, and the adjoint index $a$ ranges over $(1, \cdots, N^2 - 1)$. We assume a vanishing $\theta$ parameter multiplying the anomaly term $F \tilde{F}$.

After renormalization, the coupling $\alpha(\mu) \equiv g^2(\mu)/4\pi$ runs with energy scale, obeying a renormalization group equation

$$\mu \frac{\partial}{\partial \mu} \alpha(\mu) \equiv \beta(\alpha) = -b\alpha^2(\mu) - c\alpha^3(\mu) - \ldots .$$

The first two coefficients are renormalization scheme independent:

$$b = \frac{1}{6\pi} (11N - 2N_f) \quad (3)$$

$$c = \frac{1}{24\pi^2} \left(34N^2 - 10NN_f - 3\frac{N^2 - 1}{N}N_f\right) . \quad (4)$$

Asymptotic freedom requires $b > 0$ (or $N_f < 11N/2$). If in addition $c < 0$, there is an infrared stable, non-trivial fixed point $[10]$, located (to two-loop accuracy) at coupling

$$\alpha_* = -\frac{b}{c} . \quad (5)$$

Assuming that at some reference scale $\Lambda$, the running coupling has a value $\alpha(\Lambda)$ between 0 and $\alpha_*$, we then have $\alpha(\mu \ll \Lambda) \to \alpha_*$ and $\alpha(\mu \gg \Lambda) \to 0$. We can write the two-loop solution to the renormalization group Eq. (2) in the form

$$\frac{\Lambda}{\mu} = \left[\alpha_*/\alpha(\mu) - 1\right]^{-1/(ba_*)} \exp\left[-1/b\alpha(\mu)\right] , \quad (6)$$

giving $\alpha(\Lambda) = 0.7822\alpha_*$. Note that $\alpha(\Lambda)$ will vary when we change $N_f/N$.

The reliability of this result depends on whether higher order terms in the $\beta$ function can be ignored. That is guaranteed for sufficiently small $\alpha_*$; more generally, the higher order terms are renormalization scheme dependent and so can be made arbitrarily small. For such special renormalization schemes, or for larger $\alpha_*$, there could of course
be important higher order corrections to other quantities of physical interest [4]. Nevertheless, the higher-loop $\beta$ function [11] continues to display an infrared fixed point, with scheme-dependent accuracy discussed below.

In Ref. [9], it was argued that gluon exchange triggers dynamical chiral symmetry breaking when the fixed-point coupling $\alpha_*$ exceeds a critical value

$$\alpha_c = \frac{\pi}{3C_2(R)} = \frac{2\pi N}{3(N^2 - 1)}. \tag{7}$$

This happens when $N_f$ drops below the critical value for gluon exchange,

$$N_f^{cG} = N \left( \frac{100N^2 - 66}{25N^2 - 15} \right) \approx 4N(1 - 0.06N^{-2} - \ldots). \tag{8}$$

The leading approximation for large $N$ is quite good even for $N = 2$.

An estimate of the higher order corrections to the gap equation driving the breaking provides some evidence [12] for the reliability of these results. For $\alpha \leq \alpha_c$, the next order corrections were found to be relatively small (less than 20%) compared to the ladder approximation. As discussed above, there could also be important corrections to the $\beta$ function when $\alpha$ is this large. Some evidence that this is the case in the MS scheme adopted here can be provided by determining $\alpha_*$ using the three-loop MS $\beta$ function [11] and setting this value equal to $\alpha_c$. For $N = 2$, this leads to a new value of $N_f^{cG}/N \approx 3.175$, again shifted less than 20% from the two-loop value 3.929. The shift decreases to about 15% as $N \to \infty$.

For $N_f < N_f^{cG}$ the gap equation gives a dynamical mass $\Sigma(p)$, where $p$ is the magnitude of Euclidean momentum. It has some value $\Sigma(0)$ at $p = 0$ and then falls monotonically with increasing $p$. The scale $\Sigma(0)$ vanishes continuously in a characteristic exponential fashion [1] as $N_f \to N_f^{cG}$ from below (equivalent to $\alpha_* \to \alpha_c$ from above), at fixed $\Lambda$. Since the fermions decouple for $p \ll \Sigma(p)$, the infrared fixed point is only an approximate feature of the theory, useful at momentum scales above the decoupling scale. Fortunately, the critical behavior of the theory near the transition is determined mainly by the momentum range $\Sigma(p) \ll p \ll \Lambda$ in the gap equation integration, where the fixed point is a good approximation. Further discussion of the gluon-induced critical behavior may be found in Refs. [9, 13, 14].

Turning now to our study of the role of instantons in the chiral phase transition, we will derive a corresponding critical coupling or critical number of flavors $N_f^{cI}$, arising purely from instanton effects. Comparison with the values from purely gluon exchange will then indicate the relative importance of the two effects in the phase transition dynamics.

A nonzero dynamical mass $\Sigma(p)$ in the quark propagator $i/[A(p)\gamma_\mu p^\mu - \Sigma(p)]$ signals chiral symmetry breaking. To determine this two-point function we adopt a formalism [6] which self-consistently sums the effects on a fermion propagating through a dilute gas
of noninteracting instantons, giving a gap equation whose kernel is directly related to the single-instanton amplitude. For general \(N\), the gap equation takes the form

\[
\Sigma(p) = \int_0^\infty \frac{d\rho}{\rho^2} \rho \Gamma[\alpha(\rho)] \frac{D[\rho m(\rho)]^N}{\rho m(\rho)} f^2(\rho \rho/2)
\]

(9)

with

\[
\Gamma[\alpha(\rho)] = \frac{4e^{5/6}e^{CN-\frac{B}{Nf}}}{(N-1)! (N-2)!} \left[ \frac{2\pi}{\alpha(\rho)} \right]^{2N} e^{-2\pi/\alpha(\rho)}. \]

(10)

The numerical factors and \(\alpha\) dependence in \(\Gamma[\alpha(\rho)]\) arise from the amplitude for an instanton of size \(\rho\), integrated over the other collective coordinates \([2, 15]\). Gauge field and quark fluctuations around the instanton background contribute quantum corrections which include logarithms that renormalize the bare coupling to its value at length scale \(\rho\). Depending on the order of the calculation, we end up with the one- or two-loop renormalization group solution for \(\alpha(\rho)\), with leftover non-logarithmic terms going into the numerical prefactor.

If the two-loop \(\alpha(\rho)\) is to be used, to make use of the infrared fixed point, then the constants \(B\) and \(C\) should be computed to the same order. They have so far been computed only through one loop \([2, 15]\), where they are \(B = 0.3595\) and \(C = 2.0706\) in the MS scheme.\(^1\) The higher-order fluctuations that generate two-loop running in \(\exp(-2\pi/\alpha)\) and one-loop running \([16]\) in \((2\pi/\alpha)^{2N}\) also contribute corrections of \(\mathcal{O}(\alpha)\) to \(B\) and \(C\). We expect that a full two-loop calculation will be scheme independent. In the absence of such higher order computations, we will simply take \(\alpha(\rho)\) everywhere in the gap equation to be governed by the two-loop \(\beta\) function and infrared fixed point. For our numerical study, we will use the one-loop, MS values of \(B\) and \(C\), assuming that the higher order corrections will lead only to \(O(1)\) changes, in particular keeping \(e^B \sim \mathcal{O}(1)\).

The function \(D[\rho m(\rho)]\) contains the mass-dependent factors from the fermionic quantum fluctuations (left over after the factors containing regulated divergences are absorbed into \(\Gamma[\alpha(\rho)]\)). Following Ref. \([3]\) we evaluate the argument of \(D[\rho m(\rho)]\) using the function \(m(\rho)\) derived from \(\Sigma(p)\) weighted by the fermion zero mode wavefunction,

\[
m(\rho) = \langle \psi_0 | \Sigma | \psi_0 \rangle = \int_0^\infty dx x f^2(x/2) \Sigma(p=x/\rho).
\]

(11)

Here, \(f(x)\) is a combination of modified Bessel functions \([17]\) arising from the Fourier transform of \(\psi_0(x)\),

\[
f(x) \equiv -2I_1(x)K_1(x) - 2x(I_1(x)K_0(x) - I_0(x)K_1(x)),
\]

(12)

normalized to \(f(0) = 1\). Its asymptotic behavior is \(f(x \gg 1) \sim \frac{3}{16}x^{-3}\).

For arguments \(\rho m(\rho) \ll 1\), the fermion fluctuation factor \(D[\rho m(\rho)]\) has the expansion \(D(x) = x + \mathcal{O}(x^3 \ln x)\). For large arguments, the fermions decouple and \(D[\rho m(\rho)]\)

\(^1\) In the MS-bar scheme these become \(B = -0.2917\) and \(C = -1.5114\).
exponentially approaches unity \[18\], which we must multiply by \(e^{B} \sim \mathcal{O}(1)\) to account for decoupling the fermion factors in \(\Gamma(\alpha)\). Lacking a full calculation of the instanton determinant for massive fermions, we adopt a simple form that interpolates between these two limits:

\[
D(x) \equiv \begin{cases} 
  x & \text{for } x < e^{B} \\
  1 \cdot e^{B} & \text{otherwise} 
\end{cases}
\]  

(13)

Spontaneous chiral symmetry breaking corresponds to the existence of nonvanishing, energetically preferred solutions to the gap equation \([9]\). We will first qualitatively discuss the existence of these solutions and then summarize the results of a numerical study. To begin, we note that a nonvanishing solution \(\Sigma(p)\) will have some finite value \(\Sigma(0)\) at \(p = 0\), and then decrease monotonically. This behavior, typical for a dynamical mass in a gauge field theory, follows from the structure of the gap equation \((9)\) with the factor \(f_{2}(\rho / 2)\) decreasing monotonically from unity. The zero mode mass in Eq. \((11)\) is approximately \(m(\rho) \sim \Sigma(1/\rho)\), since \(xf^{2}(x/2)\) is peaked around \(x = 1\) and integrates to unity. Thus, \(m(\rho \to \infty) = \Sigma(0)\), while \(m(\rho)\) falls rapidly as \(\rho \to 0\). Although the intrinsic scale \(\Lambda\) sets the solution scale \(\Sigma(0)\), our interest here is in exploring a possible second order phase transition near which the gap equation may dynamically enforce \(\Sigma(0) \ll \Lambda\).

Assuming this to be the case, the integration over \(\rho\) then breaks naturally into three regimes. The ultraviolet regime, \(0 < \rho < 1/\Lambda\), contributes very little to the integral because asymptotic freedom ensures a strong suppression of \(\Gamma(\alpha(\rho))\), while \(D(\rho m)^{N_{f}}\) also remains small. In the intermediate regime, \(\Lambda^{-1} < \rho \lesssim \Sigma(0)^{-1}\), \(\alpha(\rho)\) ranges only from roughly \(0.78\alpha_{*}\) to \(\alpha_{*}\), and the infrared fixed point dominates the behavior. The upper end of this intermediate regime, \(\rho \approx \Sigma(0)^{-1}\), should dominate the integral due to the polynomial increase of \(D[\rho m(\rho)]\) while \(\Gamma(\alpha(\rho))\) simply approaches its fixed point value \(\Gamma_{*}\). In the third regime, as \(\rho \gg \Sigma(0)^{-1}\) the fermions decouple from the fluctuations, ending the polynomial increase of \(D[\rho m(\rho)]\) and the fixed point behavior of \(\alpha\). The third regime will affect the critical value of \(N_{f}\) but not the qualitative behavior near criticality.

We can see this by scaling to dimensionless variables \(s(y) = \Sigma(0)^{-1}m(y/\Sigma(0))\) with \(y = \Sigma(0)\rho\); note that \(0 \leq s(y) \leq 1\). The gap equation at \(p = 0\) then becomes

\[
1 \approx 0 + \Gamma_{*} \int_{\Sigma(0)/\Lambda}^{1} \frac{dy}{y^{2}} [ys(y)]^{N_{f} - 1} + \int_{1}^{\infty} \Gamma(y) e^{BN_{f}} \frac{dy}{y^{3}s(y)} \]  

(14)

for nonvanishing \(\Sigma(0)\). Thus it is the intermediate regime that controls the critical behavior of \(\Sigma(0)/\Lambda\). An important feature of Eq. \((14)\) is that since \(s(y) \leq 1\), it cannot be satisfied if \(\Gamma_{*} \ll 1\), which occurs for \(N_{f}\) close enough to \(11N/2\) (that is, small \(\alpha_{*}\)). Only the chirally symmetric solution \(\Sigma(0) = 0\) exists for this range of \(N_{f}\).

As we decrease \(N_{f}\) to \(N_{f}^{cl}\) (the critical number of flavors for the instanton kernel), \(\Gamma_{*}\) will eventually reach a critical value large enough to allow nonzero solutions. The structure of Eq. \((14)\) indicates that this will correspond to maximizing the intermediate integral, and therefore to taking its lower limit to zero. For \(N_{f}\) slightly less than \(N_{f}^{cl}\), \(\Sigma(0)/\Lambda\) must be small, indicating a continuous phase transition. We expect \(N_{f}^{cl} \gtrsim 3.7N_{c}\),
since if a critical value occurs it can only be before $\Gamma_*$ reaches its maximum as a function of $N_f$, corresponding to $\alpha_* \approx \pi/N$. We will not here determine analytically the behavior of $\Sigma(0)$ as $N_f \to N_f^{cf}$. Instead, having qualitatively seen that there exists a continuous phase transition at a critical value $N_f^{cf}$, we now turn to a numerical study of the transition.

The numerical results reported in this letter are restricted to the case $N = 2$. We solve Eq. (3) on a one dimensional lattice, iteratively relaxing the discretized $\Sigma(p)$ from an initial guess to a self-consistent shape, at each stage numerically integrating to get $m(\rho)$. We expect, from our qualitative discussion, that the dominant range of integration will be approximately $\Lambda^{-1} < \rho < \Sigma(0)^{-1}$. We use the exact solution Eq. (6) to the two-loop renormalization group equation, for all $\rho < \Sigma(0)^{-1}$ (more precisely, for $\rho$ below the value at which $D(\rho m) = e^B$, solved for at each iteration), using the MS value $B = 0.3595$. For $\rho$ above this fermion-decoupling value, we match $\alpha(\rho)$ onto the $\beta$ function solution for $N_f = 0$. After $\alpha$ finally grows too large for perturbative running, we simply fix it at a constant value $\alpha_{\text{max}} = 2\pi/N$; the far end of the infrared range of integration is safely subdominant, and we have checked that this approximation is unimportant.

The result is a shape $\Sigma(p)$ for each value of $N_f$. To study a possible phase transition we examine the behavior of $\Sigma(0)$, for fixed $\Lambda$, while varying $N_f$. The numerical results confirm the qualitative discussion above: when $N_f$ approaches the critical value $N_f^{cf} \approx 4.77N \approx 9.54$ from below, $\Sigma(0)$ vanishes continuously in the manner of a second order phase transition. Fig. 1a displays this behavior for $N = 2$; in contrast to the exponential behavior arising from gluon exchange, Fig. 1b indicates a power law behavior.

The critical coupling and $N_f^{cf}$ for an instanton kernel are numerically very similar to the values for the gluon-exchange kernel, basically independent of whatever $O(1)$ values are chosen for $B$ and $C$. In any case, a more complete calculation which combined the two kernels would lead to a somewhat smaller combined critical coupling (or larger critical
Finally, we discuss the validity of the dilute gas approximation, incorporated in the gap equation used here to describe the phase transition. It allows the amplitude for a fermion propagating in the field of a single instanton to be summed over multi-instanton configurations, neglecting instanton interactions. The validity of this approximation depends on the relative magnitude of the dominant instanton size and the typical separation distance between instantons in multi-instanton configurations. As noted above, the dominant instanton size is of order $\Sigma(0)^{-1}$, which grows without bound near the critical point. But the average instanton separation does just the same, since it is controlled by essentially the same instanton amplitude integral, also dominated near $\rho \sim \Sigma(0)^{-1}$.

Crudely estimating the instanton density by

$$\bar{n} \sim \int_0^\infty \frac{\rho}{\rho^5} \frac{\Gamma[\alpha(\rho)]}{2\pi^2} D[\rho m(\rho)]^{N_f} \sim \Sigma(0)^4 \frac{\alpha^{B N_f}}{2\pi^2}, \quad (15)$$

we ask that there be fewer than one instanton per instanton four-volume $\Sigma(0)^{-4}$:

$$\frac{2e^{5/6}}{\pi^2} \frac{e^{CN}}{(N-1)!(N-2)!} \left[ \frac{2\pi}{\alpha_s} \right]^{2N} e^{-2\pi/\alpha_s} \ll 1 \quad (16)$$

For $N = 2$ this requires $\alpha_c$ only slightly smaller than $\pi/N$, that is $N_f^{ci} > 26N/(7-N^{-2}) \approx 3.7N$. Our numerical result for $N = 2$ is on the safe side of this limit, giving some reassurance that instanton overlap does not violate the dilute gas approximation. For larger $N$, the non-overlap condition (16) becomes

$$\frac{e^{5/6}}{\pi^3} N^2 \left[ \frac{e^{CN/2}}{N\alpha_s} e^{1-\pi/N\alpha_s} \right]^{2N} \ll 1 \quad (17)$$

putting a somewhat stricter bound on $\alpha_c$ and $N_f^{ci}$.

It is clear from this last expression that at large $N$ the validity of the dilute gas approximation becomes a delicate matter depending sensitively on the value of $\alpha_s$, and also on $B$ and $C$. If $C$ were neglected in Eq. (17), the remaining expression would increase exponentially with $N$, for $\alpha_s$ in the range required to trigger chiral symmetry breaking. Since the same factor appears in the instanton amplitude entering the gap equation, the increase would also affect the dynamics of chiral symmetry breaking. That is, the effect of instantons would grow with $N$, at least up to the point where the dilute gas approximation breaks down. Whether this actually happens depends on the prefactor term involving $B$ and $C$. Until these constants are computed through two loops and demonstrated to be scheme independent for $\alpha(\rho) = \alpha_s$, the relevance of instantons to chiral symmetry breaking remains uncertain in the large $N$ limit.

In summary, we have studied the role of instantons in the zero-temperature chiral phase transition in $SU(N)$ gauge theories, using the number $N_f$ of fermion flavors as the control parameter. The key feature of these theories is that for a range of $N_f$ including
the critical value for the transition, the two-loop $\beta$ function exhibits an infrared fixed point. This allowed us to discuss qualitatively the existence and behavior of solutions to a gap equation, whose kernel arose from the propagation of fermions in an instanton background in the dilute gas approximation, and to present numerical solutions. We found a critical value of $N_f$, below which chiral symmetry breaking occurs, which is comparable to that generated by gluon exchange alone. We conclude that for small $N$, instantons play a role comparable to that of gluon exchange in the chiral phase transition.

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