Reliable Semiclassical Computations in QCD

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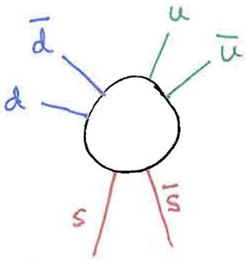
Motivation: The Strong CP Problem and $m_u = 0$

There are three plausible solutions to the strong CP problem.

1. Axions
2. Spontaneous CP Violation (Nelson-Barr mechanism)
3. $m_u = 0$.

The last seems, at first, inconsistent with current algebra estimates of meson masses. But, as pointed out by Kaplan and Manohar, this may be naive (earlier work: MacArthur and Georgi, others).



$\bar{d}$
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This can be understood naively by thinking about instanton effects in QCD. If $m_u = 0$ at, say, 100 GeV, then instanton corrections generate a u quark mass of order

$$m_u = \frac{m_d m_s}{\lambda}. \qquad (1)$$

where λ is an infrared cutoff. If $\lambda = \Lambda_{qcd}$, this is not much different than the standard m_u.

Suppose, for a moment, that this is consistent with observed facts of strong interactions. One can ask: how plausible is it that $m_u = 0$. After all, $m_u = 0$ is not protected by any (non-anomalous) symmetry.

But in response:

1. The same objection can be raised for the axion.
2. As for the axion, one can find explanations for a symmetry violated only (or more precisely dominantly) by QCD.
   - In string theory, anomalous *discrete* symmetries common. Could forbid m_u. Broken only by stringy instantons, low energy effects like QCD.
   - Models of quark masses (Leurer, Nir, Seiberg) often make such a prediction.

We don't know how to calculate this effective u quark mass analytically in QCD. Equivalently, we don't have an analytic method to determine the quark masses at some high scale. But in principle, these masses can be obtained from lattice gauge theory.

With improvements in computing power and algorithms for handling fermions, results for quark masses have been obtained, especially by the MILC collaboration. For our purposes the most important is the m_u, which is *at least seven standard deviations from zero*.

Using the two-loop perturbative calculation of the mass renormalization constant Z_m (Mason *et al.*, 2006),[11] absolute quark masses can be found,

$$
\begin{aligned}
m_s &= 88(0)(3)(4)(0)\ \text{MeV},\\
\hat{m} &= 3.2(0)(1)(2)(0)\ \text{MeV},\\
m_u &= 1.9(0)(1)(1)(1)\ \text{MeV},\\
m_d &= 4.6(0)(2)(2)(1)\ \text{MeV}.
\end{aligned}
\tag{139}
$$

The errors are statistical, lattice systematic, perturbative, and electromagnetic (from continuum estimates). Non-perturbative computations of Z_m are in progress.

Table of quark masses from " Nonperturbative QCD simulations with 2+1 flavors of improved staggered quarks", A. Bazavov et al, *Reviews of Modern Physics*, Spring 2010. $a = 0.06$ Fm(?). ($q \approx 3$ GeV).

This subject is not without controversy. Just today on the arXiv:

Quark mass dependence of two-flavor QCD

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Abstract

I explore the rich phase diagram of two-flavor QCD as a function of the quark masses. The theory involves three parameters, including one that is CP violating. As the masses vary, regions of both first and second order transitions are expected. For non-degenerate quarks, non-perturbative effects cease to be universal, leaving individual quark mass ratios with a renormalization scheme dependence. This raises complications in matching lattice results with perturbative schemes and demonstrates the tautology of attacking the strong CP problem via a vanishing up quark mass.

Skepticism about “rooted, staggered fermions", extrapolations.
But I won’t address these controversies directly today.

This is a sufficiently important and dramatic claim that it is worthy of scrutiny. (I should say that if true, it will make me, Helen, many others very happy as it points towards an axion; but precisely because of this, I would like to be sure).
As always with lattice gauge theory, one would like to have a *calibration*, i.e. an estimate of errors independent of experimental facts. One would like some non-perturbative effect which one could calculate analytically and compare with simulations. The beta function at weak coupling is one such quantity. But we would like something specific to the chiral limit.

Ancient history

Instanton calculations in QCD typically ir divergent. Not surprising; a strongly coupled theory.
E.g. calculation of some quantity with dimensions of mass:

$$m = \Lambda^{b_0} \int d\rho \rho^{b_0 - 2}. \tag{2}$$

Similarly, our effective m_u:

$$m_u = \Lambda^{b_0} m_d m_s \int d\rho \rho^{b_0}. \tag{3}$$

In the bad old days, this lead to an elaborate program (Callan, Dashen and Gross) to try and use instantons as the basis of a solution of QCD. It was doomed to failure; there was no small parameter which could be the basis of any systematic approximation.

Can one calculate short distance Green's functions?

Still in these bad old days, people asked: can one calculate instanton contributions to short distance Green's functions? E.g. could one calculate such a contribution to $R_{e^+e^-}$, by computing an instanton correction to $\Pi_{\mu\nu}$ for Euclidean separations, and continue to Minkowski space. But even for short distances, one finds Π is infrared divergent. Appelquist and Shankar, Gross and Andrei, and Ellis and collaborators noticed that the *Fourier transform* of Π is infrared finite. Traces to fact that Fourier transform of instanton solution (and zero modes, etc.) behaves as

$$e^{-p\rho}$$

. Typical results fall as high powers of momentum.

Typical expression (schematic):

$$\langle J_\mu(x_1) J_\nu(x_2)\rangle \sim (g_{\mu\nu}\partial^2 - \partial_\mu\partial_\nu) \tag{4}$$

$$\times \int d\rho \Lambda^{b_0} \rho^{b_0-1} \frac{d^4x^0}{[(x_1-x_0)^2+\rho^2]^2[(x_2-x_0)^2+\rho^2]^2}$$

For large ρ, this behaves as $d\rho\rho^{b_0-5}$ (diverges unless $n_f > 9$).

Suggests a lattice calibration. Calculate momentum space Green's functions which have *no perturbative contribution*, and take Fourier transform. E.g., in three flavor, massless QCD:

$$\Delta(x) = \langle \bar{u}(x) u(x) \bar{d}(0) d(0) \bar{s}(0) s(0) \rangle. \tag{5}$$

Fourier transform will behave as:

$$\Delta(p) = \frac{\Lambda^9}{p^5}. \tag{6}$$

Very rapid fall off with momentum, so probably impossible in practice. But proof of principle?

What can we actually calculate?

Finiteness is fine, but are these actually the dominant contributions to anything?

Why can't we calculate quantities at short distances?

Organize using the language of the *operator product expansion*.

Start with QCD with two flavors. Consider the operator:

$$\bar{u}(x)u(x)\bar{d}(0)d(0) \tag{7}$$

In perturbation theory, the leading term on the right hand side is non-singular,

$$\bar{u}(x)u(x)\bar{d}(0)d(0) \sim (1 + \mathcal{O}(\alpha_s(x)))\,\bar{u}(0)u(0)\bar{d}(0)d(0) \tag{8}$$

The matrix elements of the operator $\bar{u}(0)u(0)\bar{d}(0)d(0)$ are infrared divergent in an instanton background. This is the origin of the ir divergence in this correlation function, even at short distances.

In momentum space, this translates to $1/p^4$.
If claiming to isolate an instanton effect, would require $1/p^a$, $a < 4$.

The unit operator

Beyond perturbation theory, the unit operator can appear in the expansion. Consider N colors, N_f flavors. Study maximally chirality violating Green's function:

$$\Delta(x) = \langle \prod_{f=1}^{N_f - A} \bar{q}_f(x) q_f(x) \prod_{f=N_f-A+1}^{N_f} \bar{q}_f(0) q_f(0) \rangle \quad (9)$$

OPE

$$\prod_{f=1}^{N_f-A} \bar{q}_f(x) q_f(x) \prod_{f=N_f-A+1}^{N_f} \bar{q}_f(0) q_f(0) = C(x) + D(x) \prod_{f=1}^{N_f} \bar{q}_f(0) q_f(0) \quad (10)$$

$D(x)$ has the form $1 + a\alpha_s(x)$; it is logarithmically singular in perturbation theory. It's Fourier transform behaves as $1/p^4$.
If generated by instantons $C(x)$ has the form

$$C(x) \approx \Lambda^{11/3N-2/3N_f} |x|^{11/3N-11/3N_f}. \quad (11)$$

So power law singularity if $N_f > N$, non-singular (i.r. divergent) if $N_f < N$, borderline (logarithm) if $N_f = N$.
$SU(2)$ with three flavors first interesting (singular at short distances) case.

Momentum space:

$$C(p) \sim \Lambda^{11/3N - 2/3N_f}|p^{-4} p^{(11/3N_f - 11/3N)} \qquad (12)$$

Lesson: if instanton contributions are to dominate, the coefficient of the unit operator in the OPE must be singular.

Verify that infrared finite.

Fermion zero modes:

$$q^i_\alpha = \rho \frac{\sqrt{2}}{\pi} \frac{\delta^i_\alpha}{[(x-x_0)^2+\rho^2]^{3/2}}, \tag{13}$$

So

$$\Delta(x) = C \int d^4x_0 d\rho \frac{(\Lambda\rho)^{\frac{11}{3}N-\frac{2}{3}N_f} \rho^{3N_f-5}}{[(x-x_0)^2+\rho^2]^{3A}[x_0^2+\rho^2]^{3(N_f-A)}} \tag{14}$$

where C is a constant obtained from the non-zero modes, x_0 and ρ are the translational and rotational collective coordinates.

Perform the integral over x_0 using Feynman parameters:

$$\Delta(x) = C' \int d\alpha[\alpha^{3A-1}(1-\alpha)^{3(N_f-A)-1}]d\rho \frac{(\Lambda\rho)^{\frac{11}{3}N-\frac{2}{3}N_f}\rho^{3N_f-5}}{[x^2\alpha(1-\alpha)+\rho^2]^{3N_f-2}}. \quad (15$$

For large ρ:

$$\Delta \sim \int \frac{d\rho}{\rho}\rho^{\frac{11}{3}(N-N_f)}. \quad (16)$$

The integral converges for large ρ if $N_f > N$, exhibits a power law divergence for $N_f < N$, and diverges logarithmically for $N_f = N$.

Significance of the Infrared Divergences:

In the infrared divergent cases, the divergent part is identical to the (similarly ill-defined) instanton contribution to $\langle \mathcal{O}_1(0)\mathcal{O}_2(0) \rangle$. For $N_f < N$, the (cutoff) integral is non-singular for small x, corresponding to non-singular corrections to the coefficients of operators appearing in the OPE.

For the case $N_f = N$, the expression also has a logarithmic singularity for small x, indicating the appearance of the unit operator in the OPE, with a coefficient function behaving as $\log(x)$. It is necessary to define the operators appearing in these expressions at a scale M, and this introduces a mass scale both into the matrix element and into the coefficient of the unit operator.
We see that the coefficient of the unit operator is proportional to a single power of a logarithm. We will see that the unit operator dominates, but only by a fractional power of a logarithm.

Systematic approximation for small x

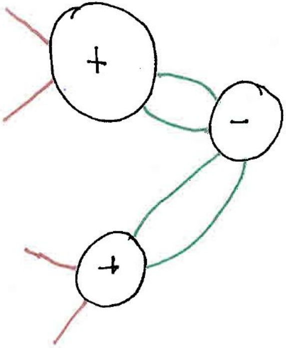
Two types of contributions to Δ:

1. Perturbative corrections to the instanton: For $N_f > N$, the contributions to the unit operator are infrared finite. Controlled by $\alpha_s(x)$.

$$e^{-\frac{8\pi^2}{g^2(x)}} \left(1 + \sum c_n \alpha_s(x)^n\right) . \tag{17}$$

2. Dilute gas contributions to the leading instanton result: These are infrared divergent, but the divergence, again, is a contribution to the matrix elements of higher dimension operators.

So calculation is systematic.



Dilute gas corrections to the single instanton result

For $N_f = N$ at best the instanton wins (or loses) by a power of a logarithm. Compute the anomalous dimensions of the various operators appearing in the OPE.
$SU(2)$ with two flavors. Take as basis of dimension six operators

$$\mathcal{O}_1 = \bar{u}u\,\bar{d}d \quad \mathcal{O}_2 = \bar{u}\sigma^{\mu\nu}u\,\bar{d}\sigma_{\mu\nu}\bar{d} \tag{18}$$

the matrix of anomalous dimensions is:

$$\Gamma = A \begin{pmatrix} 15/2 & -2 \\ 0 & 3/2 \end{pmatrix} \tag{19}$$

$$A = \frac{g^2}{16\pi^2}\frac{2}{\epsilon}. \tag{20}$$

Γ has eigenvalues

$$\gamma_1 = \frac{15}{2} A \quad \gamma_2 = \frac{3}{2} A. \tag{21}$$

Correspondingly, given that the β function in this theory is 6, at small x, relative to the unit operator contribution, $\ln(x)$, the contributions of the first operator behaves as $(\log x)^{15/12}$, while those of the second behave as $(\log x)^{1/4}$. So it is necessary to choose Green's functions carefully so as to obtain just the contribution of the second eigenoperator.

In $SU(3)$, the matrix Γ is 3×3; again, there is one operator which diverges more slowly at small x than the contribution of the unit operator. In order to isolate an instanton contribution, it is necessary to take a linear combination of operators in the Green's function, $\Delta(x)$, which projects on this.
Would be challenging in a lattice computation.

Applications to Lattice Gauge Theory

Real lattice computations: finite quark masses ($m_q \geq 10$ MeV). So correlation functions like Δ receive contributions already in perturbation theory. It is necessary that quark masses be very small if the instanton computation is to dominate.
E.g. $SU(2)$ with three flavors:

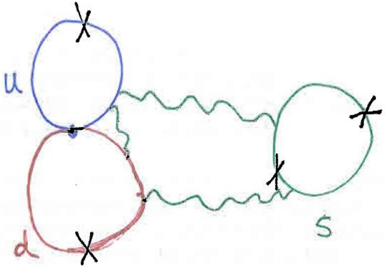
$$\langle \mathcal{O}_1(x)\mathcal{O}_2(0)\rangle = C\frac{\Lambda^{16/3}}{x^{11/3}}(1+\mathcal{O}(\alpha_s(x))). \tag{22}$$

where

$$C = 9\times 10^3 \quad \Lambda^{16/3} = \mu^{16/3} e^{\frac{-8\pi^2}{g^2(\mu)}} \tag{23}$$

in the $\overline{MS}$ scheme.

With finite quark mass, helpful to consider operators with parity properties such that they have vanishing expectation values (acknowledgment to Steve Sharpe). Then leading diagrams are high loop, so suppressed both by quark masses and α_s, and seem small enough, given masses used in practice.
So tests of lattice computations seem feasible, and potentially interesting.



Feynman diagram including mass insertions giving a perturbative contribution to the correlator.
Behaves as $\alpha_s(a)^3 m_u m_d m_s a^{-3}$.

Applications to Supersymmetric Gauge Theories (in progress)

Novikov, Shifman, Vainshtein, Zakharov: (1982-) – in a program with far reaching implications, studied instanton contributions in supersymmetric gauge theories.
Prototype: $SU(2)$ gauge theory, with chiral fermions in the adjoint representation (gluinos), λ.

$$\Delta(x) = \langle \lambda(x)\lambda(x)\lambda(0)\lambda(0)\rangle \tag{24}$$

Supersymmetry implies that this correlator is independent of x. Argued that could compute at short distances. Found a finite result for the leading contribution:

$$\Delta(x) = C\Lambda^6 \tag{25}$$

Argued that there is a non-renormalization theorem, and no corrections to the result.
Argued that taking x large, by cluster, gives value of gluino condensate.

Inconsistent, however, with result obtained using arguments of Seiberg.
Calculate in theory with a single quark flavor of mass m. For small m, compute $< \lambda\lambda >$ (or Δ). Find discrepancy by a constant factor ($3/5$).
What went wrong?
Does analysis in terms of OPE provide insight?

Don't have complete answer, but some observations:

1. We have seen that short distance, by itself, does not guarantee calculability.
2. If there are infrared divergences, these can lead to order one corrections. E.g.

$$\delta\Delta = \Lambda^6 \int \frac{d\rho}{\rho} g^2 = g^2 \log(M/\lambda) \qquad (26)$$

   with λ an ir cutoff. $\lambda \propto (Me^{\frac{-8\pi^2}{g^2}})$ gives an order one correction (consistent with holomorphy).
3. Non-perturbatively (dilute gas corrections)

$$\delta\Delta = \frac{\Lambda^{nb_0+1}\bar{\Lambda}^{nb_0}}{\lambda^{2b_0}} \qquad (27)$$

   behaves like the lowest order result, up to a numerical constant.

Currently investigating in more detail, to understand the origin of the discrepancy.

Conclusions and Future Directions:

Most interesting directions involve tests of lattice gauge theory. Doing some numerical studies to assess feasibility. Hope to find a partner for these investigations.
My guess is that the theories will pass. Perhaps main reason to worry is use of staggered fermions and particularly “rooting" (taking fourth root of fermion determinant). Much work showing that this is reliable, but no rigorous argument. Domain wall fermions will be interesting in this regard.

THE END