QCD with Large Number of Quarks: Effects of the Instanton – Anti-instanton Pairs.

M. Velkovsky and E. Shuryak

Department of Physics,
State University of New York, Stony Brook, NY 11794

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Abstract

We calculate the contribution of the instanton – anti-instanton ($I\bar{I}$) pairs to the vacuum energy of QCD-like theories with $N_f$ light fermions using the saddle point method. We find a qualitative change of the behavior: for $N_f \geq 6$ it starts to oscillate with $N_f$. Similar behaviour was known for quantum mechanical systems interacting with fermions. We discuss the possible consequences of this phenomenon, and its relation to the mechanism of chiral symmetry breaking in these theories. We also discuss the asymptotics of the perturbative series associated with the $I\bar{I}$ contribution, comparing our results with those in literature.

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In pure gauge theories the tunneling between topologically distinct classical vacua (described semiclassically by instantons) are known to shift the ground state energy down, as in quantum mechanics. It is often assumed that any non-perturbative effects should do the same: e.g. the bag constant of the MIT bag model was always assumed to be positive, without much discussion. However this is no longer obvious if there are fermions in the theory. Moreover, in supersymmetric theories only positive shifts, if any, are allowed.

In order to see how transition from one regime to another may happen, Balitsky and Yung [1] considered a toy model, a quantum mechanical double-well potential coupled to a fermion field with a certain coupling constant $a$. The contribution of tunneling-antitunneling paths was found to have a complex phase proportional to $a$, which exactly flips sign at the $a$ values at which the model becomes supersymmetric.

In this work we study what happens in the QCD-like gauge theories with $N_f$ light quarks. Unlike in the toy model mentioned, in this case the instanton contribution is only a part of the nonperturbative contribution to the vacuum energy. However, there are multiple evidences (see e.g. recent review [2]) that at least for $N_f = 0 - 3$ (here and below we imply that the number of colors is $N_c = 3$) it is a very important if not dominant part. The so called “instanton liquid” model [3] picture the vacuum of those theories as a relatively dilute and uncorrelated ensemble of instantons: it reproduces many phenomenological facts about hadronic correlations functions and spectroscopy, was recently directly supported by multiple lattice studies, see e.g. [4]. With increasing temperature $T$ correlations between instantons and anti-instantons become more important, so that the random picture is no longer valid. Eventually a chiral restoration phase transition takes place, in which only strongly correlated instanton - anti-instanton pairs, or “molecules” [5] are present.

\footnote{The absolute value of also coincides with the known shift, which ensure that the method is correct.}
This idea reproduces lattice data for close-to-QCD theories ($N_f = 0 - 3$) on the position and type of the chiral phase transitions, hadronic screening masses etc.

The pattern and mechanism of the chiral symmetry breaking at larger $N_f$ is not yet understood. It is known that chiral symmetry should be restored in the vacuum above certain critical value $N^c_f$, which should be below the value where the asymptotic freedom disappears $N^c_f < N^{AF}_f = 11N_c/2$. Between them the theory is conformal due to the infrared fixed point \[6\]. Studies of the interacting instanton ensemble \[8\] have shown that instantons alone cannot support the condensate already for $N_f > 4$. Lattice simulations for $N_f = 8$ \[15\] has found at weak coupling regime a chirally symmetric phase, similar to what was recently observed for $N_f = 16$ \[14\]. Furthermore, for $N_f = 4$ \[10\] have the quark condensate was found to be nonzero but drastically smaller than for $N_f = 0 - 3$. However, estimates based on one loop gap equation \[7\] suggest much larger critical value $N^c_f \approx 11$: presumably the condensate induced by this mechanism is too small be seen in the lattice measurements mentioned.

As $N_f$ is increased, the two basic components of the instanton ensemble mentioned above, (i) “single” (uncorrelated) ones and (ii) strongly correlated $\bar{II}$ pairs or “molecules”, have the opposite trends. Singles can only exist due to nonzero value of the quark condensate. The fermionic determinant proportional to $|\langle \bar{q}q \rangle |^{\rho^3 N_f}$ suppresses small-size instantons, so that only large ones, with sizes $\rho \sim |\langle \bar{q}q \rangle |^{-1/3}$, survive\[2\].

The “molecules” do not need a nonzero quark condensate: thus they become the dominant effect. Furthermore, as noticed in \[11\], for increasing $N_f$ they move toward smaller sizes, and for $N_f > 11N_c/2 - 3$ their density even becomes ultraviolet divergent\[3\]. The differential contribution to the normalized molecular partition function

\[2\] Those are outside the semi-classical domain, unless we are close to chiral restoration boundary \[9\].

\[3\] It can be seen on purely dimensional ground: the density of molecules is $dn_m \sim d\rho \Lambda^{2b} \rho^{2b-5}$.
of instantons and anti-instantons with small (in order to use semi-classical formulae) radii $\rho_I, \rho_{\bar{I}} << 1/\Lambda$:

$$\frac{d^2 Z_{mol}}{d\rho_I d\rho_{\bar{I}}} = V^{(4)} C^2 \rho^4 \int d^4 R d\Omega (-\rho^2 |T_{II}(R, \Omega)|^2)^{N_f} \exp(-S_{int}(R, \Omega)),$$  \hspace{1cm} (1)

where $R$ is the separation in units of $\rho$ and $\Omega$ the relative orientation of the $I\bar{I}$ pair. $C$ is standard single instanton density:

$$C = \frac{4.6 \exp(-1.86 N_c)}{\pi^2 (N_c - 1)! (N_c - 2)!} \frac{1}{\rho^5} (S_0)^{2N_c} \exp(-S_0),$$  \hspace{1cm} (2)

Up to two loops the relation between the instanton action $S_0$ and size is

$$\rho = e^{-\frac{S_0}{b}} \left[ \frac{2b}{b_1} S_0 + 1 \right]^{\frac{b_1}{2b}},$$  \hspace{1cm} (3)

where $b = \frac{14}{3} N_c - \frac{2}{3} N_f$, $b_1 = \frac{34}{3} N_c^2 - \frac{14}{3} N_c N_f + \frac{N_f}{N_c}$. The so-called overlap matrix element of the Dirac operator enting here is

$$T_{II} = \int dt d^3 x \phi_I^\dagger(x - z_I, \Omega_I) \mathcal{D}_{\bar{I}}(x - z_{\bar{I}}) \phi_{\bar{I}}$$  \hspace{1cm} (4)

with $\phi$ being fermionic zero modes of the instanton and anti-instanton.

The gauge interaction $S_{int}(R, \Omega)$ in general depends on the gauge configurations used. For $\bar{I}I$ configurations one cannot use the equations of motion because there is no nontrivial minimum: one should use the Streamline equation instead $[1, 16, 12]$. However, we will only be interested in the saddle points at large enough $R$, so that well-known dipole formula would be sufficient.

The integrand in (1) has a maximum at $R \rightarrow 0$, so the integral appears to be dominated by the weak field configurations, which belong to perturbative sector. The way to separate the non-perturbative physics is to use the saddle point method, moving the contour in the complex $R$ plane $[1]$. Let us split the contour into 2 parts, one going from $R = 0$ to $R = i\infty$, corresponding to the perturbative contribution, which becomes UV divergent at $b < 2$. This phenomenon is similar to the UV divergence in the $O(3)$ $\sigma$ model: both are curious examples of the UV divergences of nonperturbative nature.
and the other one going from that point to \( R = +\infty \) in such a way that \(|R|\) is always big, so that (4) is applicable\(^4\). The second integral is identified as a non-perturbative part of \( Z_{\text{mol}} \). It is generally complex, and its imaginary part should be compensated by the perturbative contribution: thus the well known relation to perturbative series:

\[
E_k^{\text{pert}} = -\frac{1}{\pi} \int_0^\infty \frac{dg}{g^{k+1}} \text{Im}(E_{\text{non.pert}}(g)),
\]

(5)

At the saddle point there is a balance between the gauge and fermionic part of the action: therefore we treat \( N_f \) as a large parameter, which however should also be much smaller than the single instanton action \( S_0 \) in order to ensure that the saddle point is at large \( R \): \( S_0 \gg N_f \gg 1 \). If so, we may use asymptotic expressions for \( T_{II} \) and \( S_{\text{int}} \)\(^5\). Changing to variables \( \beta = 1/R^2 \) and \( \xi = \cos^2(\theta) \), where \( \theta \) is the only relevant orientation angle, (4) becomes:

\[
\frac{d^2Z_{\text{mol}}^{\text{non.pert}}}{d\ln \rho_I d\ln \rho_{\bar{I}} V^{(4)}} = C^2 \rho^6 I
\]

\[
I = \int_0^\pi d\theta \frac{\sin^2(\theta)}{\pi/2} 4\pi \int_0^{\infty} dRR^3 e^{-S_0 4(1-4\cos^2\theta)} \left( -\frac{16\cos^2(\theta)}{R^6} \right)^{N_f}
\]

\[
= 4(-16)^{N_f} \int_0^1 d\xi \frac{1}{\xi} \int_0^{\infty} \frac{d\beta}{\beta} \exp(-S_0 4\beta^2 (1 - 4\xi) + (3N_f - 2) \ln \beta).
\]

(6)

There are two saddle points at \( \beta_0 = \pm \sqrt{\frac{3N_f - 2}{8S_0(1 - 4\xi)}} \). When \( \xi < 1/4 \) they are real and we take the positive one, but for \( \xi > 1/4 \) they are imaginary. It is irrelevant which one we choose (the choice is related to the definition of the perturbation series), so we take the one in the lower complex plane. Doing the \( \beta \) integral by the steepest

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\(^4\)Presumably there are no singularities that can prevent it.

\(^5\)Note that the addition of more terms in the expansion of \( T_{II} \) and \( S_{\text{int}} \) leads to new saddle points at smaller separations. Those however are artefacts of the truncation of the asymptotic series and should be disregarded.
descent method (the answer is analytic in $\xi$), we get for (8):

$$I = 4(-16)^{N_f} \sqrt{\pi(8S_0c)} \frac{3N_f - 2}{2} (3N_f - 2) \frac{3N_f - 3}{2} \int_0^1 d\xi \sqrt{\frac{1 - \xi}{\xi}} \xi N_f (1 - 4\xi) \frac{3N_f - 2}{2} \quad (7)$$

The above integral has a singularity at $\xi = 1/4$ which can be avoided by taking $\xi$ integration over a contour in the complex plane. A contour in the upper $\xi$ plane matches the real positive $\beta_0$ for $\xi < 1/4$ to the negative imaginary one we have chosen for $\xi > 1/4$.

For even $N_f$ the integral (10) can be written as a contour integral around the cut from 0 to 1 (avoiding $\xi = 1/4$), and the contributions are from two poles: $\xi = 1/4$, which is of order $(3/2)N_f - 1$ and gives purely imaginary contribution and $\xi = \infty$, which is of order $3 - 1/2N_f$, which gives a real contribution, but ceases to exist for $N_f \geq 6$. That is where the behaviour of the integral changes. For odd $N_f$ one can express the integral via the incomplete elliptic integrals and their derivatives. In this case there are both real and imaginary contributions. Table 1. contains the values of the real and imaginary parts of $\frac{d^2E_{mol,\text{gas}}}{d\ln \rho_f d\ln \rho_f}$ in units $\Lambda$, for $N_c = 3$, for $\rho = \frac{1}{3\Lambda}$.

Table 1.

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6 It is actually an artefact, due to the truncation of $\beta = 1/R^2$ series. In fact close to that point the steepest descent method is not applicable if we truncate the gauge action to order $O(\beta^3)$, because there is no large parameter in the exponent. However the $O(\beta^4)$ term is nonzero at $\xi = 1/4$ and if we take it into account, the integral will be finite. In this case, however, we have 4 saddle points, and we have the difficulty of defining the integral so that no spurious ones contribute to it.

7 Note that for small $N_f$ the results are unreliable because the condition $N_f >> 1$ is not true; those are shown for comparison only. Note also that we have not attempted to integrate over the instanton sizes, because that cannot be done without introducing a particular assumptions about the mechanism of the cutoff at large sizes.
Here \( I(N_f) = \text{Im} \left[ \frac{\partial^2 E_{\text{mol, gas}}}{\partial \ln \rho_f \partial \ln \rho_f} \right] e^{2S_0 e^{-4N_c + (3/2)N_f - 1}} \) is the imaginary part of the energy derivative with the dependence on \( S_0 \) (respectively \( g \)) removed.

The obtained \( N_f \) dependence of the instanton–anti-instanton contribution to the partition function is very peculiar. First of all, in many cases the real part of the obtained result vanishes. Second, its signs start to oscillate for \( N_f > 5 \). Coincidentally, this is also the region where the instantons cannot support chiral condensate, and, as discussed above, their contribution is probably very small.

In this paper we have not investigated the effective interaction between fermions induced by the “molecules”, but comment that one should expect for intermediate \( N_f \) appearance of non-perturbative forces and hadronic states having two distinct scales, dictated by the condensate and “molecules”. Furthermore (at least in the saddle point approximation used in this work) their sign and magnitude of the latter should be proportional to the vacuum shifts evaluated above. As a result, the oscillatory behaviour found in this work should also propagate to correlators (at

| \( N_f \) | \( \text{Re} \left[ \frac{\partial^2 E_{\text{mol, gas}}}{\partial \ln \rho_f \partial \ln \rho_f} \right] \) | \( \text{Im} \left[ \frac{\partial^2 E_{\text{mol, gas}}}{\partial \ln \rho_f \partial \ln \rho_f} \right] \) | \( I(N_f) \) |
|---|---|---|---|
| 1 | \( .7959 \times 10^{-5} \) | \( -.1717 \times 10^{-4} \) | \( -.7173 \times 10^{-5} \) |
| 2 | 0. | \( -.5098 \times 10^{-5} \) | \( -.2690 \times 10^{-5} \) |
| 3 | \( -.3668 \times 10^{-7} \) | \( -.5474 \times 10^{-7} \) | \( -.2833 \times 10^{-5} \) |
| 4 | \( -.1917 \times 10^{-7} \) | \( -.5330 \times 10^{-8} \) | \( -.1991 \times 10^{-5} \) |
| 5 | \( -.1027 \times 10^{-7} \) | \( .6464 \times 10^{-8} \) | \( .1178 \times 10^{-4} \) |
| 6 | 0. | \( .1520 \times 10^{-7} \) | \( .7913 \times 10^{-4} \) |
| 7 | \( .5067 \times 10^{-7} \) | \( .1127 \times 10^{-7} \) | \( .7147 \times 10^{-4} \) |
| 8 | 0. | \( -.2714 \times 10^{-5} \) | \( -.2292 \times 10^{-2} \) |
| 9 | \( -.1898 \times 10^{-3} \) | \( .1368 \times 10^{-4} \) | \( .2067 \times 10^{-2} \) |
| 10 | 0. | \( .3365 \times 10^{-4} \) | .4120 |
| 11 | \( .1093 \times 10^{-6} \) | \( .2421 \times 10^{-8} \) | .1480 |
| 12 | 0. | \( -.6030 \times 10^{-11} \) | \( -132.8 \) |
sufficient small distances) and hadronic spectra.

Let us now evaluate the large order coefficients in the perturbation series due instanton–anti-instanton contribution. Using (7) we can find the energy:

\[
\frac{d^2 E_{k}^{\text{pert}}}{d \ln \rho_1 d \ln \rho_2} \rho^4 = \frac{1}{\pi} \int \frac{dg}{g^{k+1}} \frac{8\pi^2}{g^2} e^{-\frac{16\pi^2}{3} I(N_f)}
\]

\[
= -I(N_f) \frac{1}{2\pi} \left( \frac{1}{8\pi^2} \right)^{k/2} \int_0^\infty d(S_0) (S_0)^{4N_c-(3/2)N_f+k/2} e^{-2S_0},
\]

This is yet another saddle point integral with a saddle point at \( S_0 = 2N_c - 3/4N_f + k/4 \). The applicability condition now is \( k >> 3N_f \). Finally we get the expected factorial behaviour:

\[
\frac{d^2 E_{k}^{\text{pert}}}{d \ln \rho_1 d \ln \rho_2} \rho^4 = -I(N_f) \sqrt{\frac{1}{4\pi}} \left( \frac{1}{8\pi^2} \right)^{k/2} \times
\]

\[
\left( \frac{4N_c - (3/2)N_f + k/2}{2} \right)^{4N_c-(3/2)N_f+k/2+1/2} e^{-(4N_c-(3/2)N_f+k/2)}
\]

\[
= -I(N_f) \frac{1}{2^{4N_c-(3/2)N_f}} \left( \frac{1}{4\pi} \right)^{k+1} \Gamma(4N_c-(3/2)N_f + k/2 + 1).
\]

One can compare it with the results for the \( \bar{II} \) contribution to cross section of the process of \( e^+e^- \rightarrow \text{hadrons} \). In [18] the factorial behavior is \((4N_c + k/2)!\) for \( N_f = N_c = 3 \). In [19] for the standard choices of \( N_c \) and \( N_f \) the authors get

\[
R_{e^+e^-\rightarrow\text{hadrons}} = \sum -813(3280.5k)^{-35/k} (10 + k/2)! \frac{g^k}{4\pi},
\]

which is quite close to the behaviour of (11) for \( N_c = 3 \) and \( N_f = 2 \).

In summary, we have calculated the contribution of a correlated instanton–anti-instanton pair to the partition function of the QCD-like theories with increasing number of fermions. On general grounds (and the analogy to the quantum-mechanical problem with fermions) it was expected that the behaviour should have an oscillatory pattern, shifting the ground state down or upward as \( N_f \) grows. This

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8 The coefficients are smaller than those due to "renormalons", which however correspond to a completely different set of diagrams, with maximal number of loops instead of classical "trees".

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was indeed found to be true, but only for large enough $N_f$. The same is expected to happen for the hadronic spectra. Our results for the asymptotic of the perturbative series generated by $\tilde{II}$ configurations are very close to those obtained in [15, 16] by a different method.
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