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A Lorentz invariant sum rule for the θ-dependence in QCD

Hisashi Kikuchi and Josć Wudka

Department of Physics
University of California, Riverside
Riverside, CA 92521

ABSTRACT

A sum rule for the θ-dependence in QCD is derived. Special attention is paid to the subtleties associated with the translation of the Lagrangian path integral result into Hamiltonian canonical quantization language, and the Lorentz non-covariance of T-product within canonical $G_0^a = 0$ quantization. Prescriptions for dealing with these problems are given.

1. The addition to a Lagrangian of exact differentials does not affect classical motion, but can potentially (and significantly) alter the nature of the system upon quantization. In this paper we will consider the effects of such modifications restricting ourselves to the phenomenologically interesting case of CP odd terms, which we label "θ-terms"; we denote by θ the corresponding coefficient. The evaluation of the dependence of physical observables on θ within a given model is, in general, a highly nontrivial dynamical problem [1]. This is the case in QCD, where the determination of the θ dependence is a problem of both theoretical and phenomenological relevance: experimental evidence strongly suggests that observables are independent of θ, while, on the other hand, there is no theoretical understanding of this effect (within QCD) [2]. In this paper we will determine a sum rule describing the θ dependence of a model, we will first consider the case of a quantum mechanical system and then follow a similar approach for QCD.

A quantity which we will use to measure the θ-dependence in a given model is the energy density of the vacuum

$$\varepsilon(\theta) \equiv \lim_{\beta,V\to\infty} \frac{i}{\beta V} \ln Z(\theta,\beta,V), \tag{1}$$

where $Z(\theta,\beta,V)$ is the Minkowsky space partition function with time period β and space volume V. Z can be written using the Lagrangian path integral

$$Z(\theta,\beta,V) = \int [d\phi]\, e^{i\int_0^\beta dt \int_V d\vec{x}\, L_\theta[\phi]}, \tag{2}$$

where ϕ denotes the fields of the model.

Equivalently we can consider the differential coefficients at $\theta = 0$ (assuming a smooth θ dependence):

$$\varepsilon'(0) = -\langle\langle\, Q(0)\,\rangle\rangle, \tag{3}$$

$$\varepsilon''(0) = (-i)\int d^4x \left[\langle\langle\, Q(x)\,Q(0)\,\rangle\rangle - \langle\langle\, Q(0)\,\rangle\rangle^2\right], \tag{4}$$

etc., where

$$Q(x) \equiv \frac{dL_\theta}{d\theta} \tag{5}$$

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and

$$\langle\langle\, \mathcal{O} \,\rangle\rangle \equiv \lim_{\beta,V\to\infty} \frac{1}{Z(\theta,\beta,V)} \int [d\phi]\, \mathcal{O}\, e^{i\int_0^\beta dt \int_V d\vec{x}\, L_\theta[\phi]}\Big|_{\theta=0} . \tag{6}$$

These differential coefficients relate the θ-dependence of the vacuum energy density to correlation functions of the charge Q of the system at $\theta = 0$.

The relevance of the Eqs. (3)-(4) becomes more transparent when rewritten in terms of field operators. Then, by inserting a complete set of eigen-states of the Hamiltonian as intermediate states, we can, in principle, evaluate $\varepsilon'(0)$, $\varepsilon''(0)$, etc. in terms of a sum over appropriate matrix elements of $Q(x)$. These expressions can then be regarded as sum rules describing the θ-dependence of the system.

When translating the path integral result into canonical operator language, the naive interpretation of the correlation function $\langle\langle\, \mathcal{O} \,\rangle\rangle$ as the vacuum expectation value of the T-product $\langle 0|\, \mathrm{T}\, \mathcal{O}\, |0\rangle$ is not correct: contact terms must be added [3] (see also Ref. [4]). As we will show below, the existence of these contact terms resolves an apparent contradiction related to the θ-dependence of the vacuum energy in quantum mechanical systems. Within field theory this solution is still not satisfactory: the result does not appear to be Lorentz invariant, although $\varepsilon(\theta)$ and all its differential coefficients must be Lorentz scalar. Indeed, the Euclidean version of $Z(\theta)$ corresponds to the zero temperature gluonic partition function (with zero chemical potential), $\varepsilon(\theta)$ can then be interpreted as minus the vacuum pressure, which is a Lorentz scalar. This implies that the vacuum expectation value of energy momentum tensor is given by $\langle 0|T^{\mu\nu}|0\rangle = \varepsilon(\theta)\, g^{\mu\nu}$.

In this paper, we solve this paradox and write down the sum rules for $\varepsilon'(0)$, $\varepsilon''(0)$, etc. in a manifestly Lorentz invariant fashion. For definiteness we concentrate on the second differential coefficient $\varepsilon''(0)$, the extension for the higher coefficients is straightforward (the first differential coefficient is zero in QCD due to time reversal symmetry). We divide the calculation into two steps. First, using the Hamiltonian path integral, we establish

a translation rule between the Lagrangian path integral expression for the correlation functions and the canonical operator language Green's functions. Second, we covariantize the results by replacing the T-products with T*-products which entails the evaluation of the corresponding seagull terms.

2. We begin by considering the case of one-dimensional field theory (quantum mechanics) since it provides an instructive and transparent example both for obtaining the translation rule, and for understanding Eq. (3)-(4) as sum rules. We consider a particle moving in a potential $V(x)$,

$$L_\theta = \frac{1}{2}\dot{x}^2 - V(x) + \theta\dot{x}. \tag{7}$$

The path integral expression of $\varepsilon''(0)$ is

$$\varepsilon''(0) = (-i) \int dt\, \langle\langle\, \dot{x}(t)\, \dot{x}(0)\, \rangle\rangle, \tag{8}$$

where we used $\langle\langle\, \dot{x}(0)\, \rangle\rangle = 0$, a simple consequence of time reversal invariance at $\theta = 0$.

The corresponding Hamiltonian is

$$H_\theta = \frac{1}{2}(p-\theta)^2 + V(x) \tag{9}$$

and Heisenberg equation for operator $x(t)$ is $\dot{x}(t) = p(t)$ for $\theta = 0$.

Now, can we replace $\dot{x}(t) \to p(t)$ and $\langle\langle \ldots \rangle\rangle \to \langle 0|\, \mathrm{T} \ldots |0\rangle$ in Eq. (8)? The answer for this question is "**No.**" Indeed, if we adopt this naive translation rule, we find a contradiction: writing $\varepsilon''(0)$ as the zero frequency limit of the relevant Fourier transform we obtain the inequality

$$\varepsilon''(0) \stackrel{?}{=} \lim_{\omega\to 0}(-i) \int dt e^{i\omega t} \langle 0|\, \mathrm{T}\, p(t)\, p(0)\, |0\rangle = \lim_{\omega\to 0} \int_0^\infty dm \frac{2m\, \rho_c(m)}{\omega^2 - m^2 + i\epsilon} < 0 \tag{10}$$

by virtue of the positiveness of the (connected) spectral function

$$\rho_c(m) \equiv \sum_{n\neq 0} |\langle 0|\, p(0)\, |n\rangle|^2\, \delta(m - E_n + \varepsilon(0)), \tag{11}$$

where $|n\rangle$ are the eigen-states of H_0 with corresponding eigen-values E_n. This inequality, however, is false for periodic potentials for which it is known [5] that $\varepsilon(\theta) \sim \alpha(1-\cos\theta)$, $\alpha > 0$ which implies $\varepsilon''(0) > 0$. This shows that the naive translation rule is incorrect.

To find the correct correspondence between the path integral and operator expressions for the correlation functions, we consider the expression for Z in terms of a Hamiltonian path integral with canonical variables x and p

$$\begin{aligned} Z(\theta,\beta) &= \langle 0|\, e^{-iH_\theta\beta}\, |0\rangle \\ &= \int [dp][dx] \exp\left[-i\int_0^\beta dt\{H_\theta[p,x] - \dot{x}p\}\right], \end{aligned} \tag{12}$$

where the functional integral is over two independent functions $x(t)$ and $p(t)$; integrating over $p(t)$ and using Eq. (7) we recover Eq. (2). Substituting (12) in (1) and using (9) we obtain

$$\varepsilon''(0) = 1 - i\int dt \langle\!\langle\, p(t)\, p(0)\, \rangle\!\rangle. \tag{13}$$

Noting that

$$\left(p - i\frac{\delta}{\delta p}\right) i\int dt\ (p\dot{x} - H_0) = \dot{x} \tag{14}$$

we find that the correct correspondence is

$$\dot{x} \to p - i\frac{\delta}{\delta p}. \tag{15}$$

For example

$$\begin{aligned} &\langle\!\langle\, \dot{x}(t)\, \dot{x}(0)\, \rangle\!\rangle \\ &= \frac{1}{Z}\int [dp][dx] \left(p(t) - i\frac{\delta}{\delta p(t)}\right)\left(p(0) - i\frac{\delta}{\delta p(0)}\right) e^{i\int_0^\beta dt\{\dot{x}p - H_0\}} \\ &= i\delta(t) + \langle\!\langle\, p(t)\, p(0)\, \rangle\!\rangle. \end{aligned} \tag{16}$$

Once we write the correlation function in terms of $x(t)$ and $p(t)$ by eliminating all $\dot{x}$ factors, the translation to canonical operator is straightforward.

The translation rule (15) can be stated as follows: " In replacing $\dot{x}(t)$ with $p(t)$, check if there is a $p(t')$ factor in the correlation function. If present, add a contact term generated by replacing $p(t')$ and $\dot{x}(t)$ with $i\delta(t'-t)$. Repeat until all $\dot{x}$ factors have been replaced."

We also note that by the construction of (12) using time slicing, the correlation functions obtained using (15) to eliminate $\dot{x}$ in favor of p will correspond to the T product Green's functions.

The correct sum rule for $\varepsilon''(0)$ is now given by

$$\varepsilon''(0) = 1 - i\int dt\, \langle 0|\, \mathrm{T}\, p(t)\, p(0)\, |0\rangle = 1 - \int_0^\infty dm\, \frac{2\,\rho_c(m)}{m}. \tag{17}$$

For the harmonic oscillator potential $V(x) = x^2/2$ we obtain $\rho_c(m) = \delta(m-1)/2$ and thus $\varepsilon''(0) = 0$, a result consistent with the absence of any θ-dependence in this case.

Note also that Eq. (17) can be rewritten as

$$\varepsilon''(0) = -i\int dt\, \frac{d}{dt}\langle 0|\, \mathrm{T}\, x(t)\, p(0)\, |0\rangle. \tag{18}$$

Thus a nontrivial θ-dependence, $\varepsilon''(0) \neq 0$, indicates the presence of long time correlations between x and p.

We now apply the same analysis to QCD. The Lagrangian reads [1]

$$L_\theta = -\frac{1}{4}G^a_{\mu\nu}G^{a\mu\nu} + \theta\frac{g^2}{32\pi^2}G^a_{\mu\nu}\tilde{G}^{a\mu\nu}, \tag{19}$$

where

$$G^a_{\mu\nu} = \partial_\mu G^a_\nu - \partial_\nu G^a_\mu + g f^{abc} G^b_\mu G^c_\nu, \qquad \tilde{G}^{a\mu\nu} = \frac{1}{2}\epsilon^{\mu\nu\lambda\sigma}G^a_{\lambda\sigma}. \tag{20}$$

In this paper we will ignore the quark contributions.

Using the $G^a_0 = 0$ gauge the Hamiltonian is given by

$$H_\theta = \frac{1}{2}(\pi^a_i + \bar{\theta}B^a_i)^2 + \frac{1}{2}(B^a_i)^2; \qquad \bar{\theta} \equiv (g^2/8\pi^2)\theta, \tag{21}$$

[1] We use the same metric as that in Bjorken and Drell [6]: $g^{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$. $\epsilon_{0123} = -\epsilon^{0123} = 1$. f^{abc} denote the SU(3) structure constants.

where π_i^a is the canonical momentum conjugate to G_i^a, and $B_i^a \equiv \epsilon_{ijk} G_{jk}^a/2$ is chromo-magnetic field. The fields operators π_i^a and G_i^a are assumed to satisfy the equal time canonical commutators

$$[\pi_i^a(t,\vec{x}), G_j^b(t,\vec{y})] = -i\delta(\vec{x}-\vec{y})\delta_{ij}\delta^{ab} \tag{22}$$

and

$$[\pi_i^a(t,\vec{x}), \pi_j^b(t,\vec{y})] = [G_i^a(t,\vec{x}), G_j^b(t,\vec{y})] = 0. \tag{23}$$

Physical states are constrained by the Gauss law

$$\mathcal{D}_i \pi_i^a | \, \rangle \equiv (\partial_i \pi_i^a + g f^{abc} G_i^b \pi_i^c) | \, \rangle = 0. \tag{24}$$

The translation rule between Lagrangian path integral and operator languages is obtained from

$$\begin{aligned} Z(0) &= \int [d\pi_i^a][dG_i^a][dG_0^a] \\ &\quad \times \exp\left[-i \int d^4x \left\{ H_\theta[\pi_i^a, G_i^a] - (\mathcal{D}_i \pi_i^a) G_0^a - \pi_i^a \dot{G}_i^a \right\}\right], \end{aligned} \tag{25}$$

which is the path integral expression for the partition function in the canonical variables [7], where G_0^a has been re-introduced as a Lagrange multiplier for the constraint (24). If we perform the π_i^a integral we recover the Lagrangian path integral expression. By argument identical to those used in the context of quantum mechanics, we get the correct translation rule: "Every time we replace G_{0i}^a in the correlation function with π_i^a, we must add a contact term generated by replacing each $\{G_{0i}^a(x), \pi_j^b(y)\}$ pair with $i\delta(x-y)\delta_{ij}\delta^{ab}$."

From (19), and applying the above translation rule, we get

$$\begin{aligned} \varepsilon''(0) &= (-i)\left(\frac{g^2}{8\pi^2}\right)^2 \int d^4x \langle\langle \{G_{0i}^a(x) B_i^a(x)\} \{G_{0j}^b(0) B_j^b(0)\} \rangle\rangle, \\ &= \left(\frac{g^2}{8\pi^2}\right)^2 \left[\langle 0| B_i^a(0)^2 |0\rangle - i \int d^4x \langle 0| \mathrm{T}\, \pi_i^a(x) B_i^a(x)\, \pi_j^b(0) B_j^b(0) |0\rangle \right] \end{aligned} \tag{26}$$

for the second differential coefficient.

3. As mentioned previously $\varepsilon''(0)$ is a Lorentz invariant quantity, but the right hand side of Eq. (26) is not manifestly a Lorentz scalar. The second step in our calculation is to write Eq. (26) in a manifestly Lorentz invariant form; to this end we use the technique developed for covariantizing the T-product of fermion current operators [8, 9].

We first examine the equal time (canonical) commutator of two $\pi_i^a B_i^a$ operators. We obtain

$$\begin{aligned} &\left[\pi_i^a(\vec{x}) B_i^a(\vec{x}), \pi_j^b(\vec{y}) B_j^b(\vec{y})\right] \\ &\quad = -2i\epsilon_{ijk} \pi_i^a B_j^a\, \partial_k \delta(\vec{x}-\vec{y}) + i\epsilon_{ijk} \left[\frac{\partial}{\partial y^k} \pi_i^a(\vec{y}) B_j^a(\vec{y})\right] \delta(\vec{x}-\vec{y}). \end{aligned} \tag{27}$$

We notice the presence of a "Schwinger-like term", the first term on right hand side in Eq. (27). Thus the T-product of two $\pi_i^a B_i^a$ operators is not a Lorentz covariant object [8]. [Since $\pi_i^a B_i^a$ is a gauge invariant operator, it transforms as a Lorentz scalar, even in $G_0^a = 0$ gauge.] We therefore need a seagull term τ in order to construct the manifestly Lorentz covariant T*-product,

$$\begin{aligned} &\mathrm{T}^*\, \pi_i^a(x) B_i^a(x)\, \pi_j^b(y) B_j^b(y) \\ &\quad \equiv \mathrm{T}\, \pi_i^a(x) B_i^a(x)\, \pi_j^b(y) B_j^b(y) + i\tau(y)\delta(x-y), \end{aligned} \tag{28}$$

where the non-covariance in the T-product is cancelled by that in τ.

To determine $\tau(y)$, we re-write Eq. (27) in terms of a time like unit vector n^μ:

$$\begin{aligned} &\delta((x-y)\cdot n) \left[\pi_i^a(x) B_i^a(x), \pi_j^b(y) B_j^b(y)\right] \\ &\quad = iS^\alpha(y;n)(g_\alpha{}^\beta - n_\alpha n^\beta)\partial_\beta \delta(x-y) + iC(y;n)\delta(x-y), \end{aligned} \tag{29}$$

where $S^\alpha(y;n)$ and $C(y;n)$ are the Lorentz covariant but frame dependent (n-dependent) operators, determined by the condition that Eq. (29) reduces to Eq. (27) when $n^\mu = (1,\vec{0})$. The seagull $\tau(y)$ is given by

$$\tau(y) = \tau(y;n)|_{n^\nu=(1,\vec{0})} \tag{30}$$

where $\tau(y;n)$ is a solution of [8]

$$\frac{\partial}{\partial n_\alpha}\tau(y;n) = S^\alpha(y;n). \tag{31}$$

From Eq. (29) we find

$$S^\alpha(y;n) = -2G^a_{\beta\mu}G^{a\alpha\mu}n^\beta \tag{32}$$

where we replaced $\pi^a_i \to G^a_{0i}$. Then we get

$$\tau(y;n) = -G^a_{\beta\mu}G^{a\alpha\mu}n^\beta n_\alpha, \quad \tau(y) = \pi^a_i(y)^2. \tag{33}$$

There is an intrinsic ambiguity in the definition to the T* product corresponding to the addition of Lorentz invariant terms to τ; in fact, if we replace $\tau \to \tau + \mathcal{O} = \tau'$, where $\mathcal{O}$ is an arbitrary local Lorentz invariant operator, the Lorentz transformation properties of the T*-product remain unchanged. This affects the definition of both the seagull (33) and T*-product (28), but not the equal time commutator (29). Our choice Eq. (32) defines what we understand by T*. Using Eq. (33) and (28), we obtain

$$\varepsilon''(0) = \left(\frac{g^2}{8\pi^2}\right)^2 \Big[\langle 0|\, B^a_i(0)^2 - \pi^a_i(0)^2\, |0\rangle \\ -i\int d^4x \langle 0|\, \mathrm{T}^*\, \pi^a_i(x)B^a_i(x)\, \pi^b_j(0)B^b_j(0)\, |0\rangle\Big], \tag{34}$$

for the second differential coefficient in Lorentz invariant form.

Incidentally, the above derivation shows that the vacuum expectation value of the T-product of two $\pi^a_i B^a_i$'s is a Lorentz scalar if and only if the expectation value of $(B^a_i)^2$ is zero.

We now write Eq. (34) using a spectral representation so that its nature as a sum rule becomes clear. Let $F(p)$ denote the Fourier transform of the T*-product:

$$\begin{aligned} F(p) &\equiv \int dx e^{ipx}(-i)\langle 0|\, \mathrm{T}^*\, \pi^a_i(x)B^a_i(x)\, \pi^b_j(0)B^b_j(0)\, |0\rangle \\ &= \int dx e^{ipx}(-i)\langle 0|\, \mathrm{T}\, \pi^a_i(x)B^a_i(x)\, \pi^b_j(0)B^b_j(0) + i\pi^a_i(0)^2\delta(x)\, |0\rangle. \end{aligned} \tag{35}$$

For $x^0 \neq 0$ the T* and T-products coincide, and we can write their vacuum expectation value using a spectral decomposition. At $x^0 = 0$ the T*-product can have δ-function type singularities which are related to corresponding singularities in the T-product. By Lorentz invariance, these singularities correspond to terms in $F(p)$ which are polynomial in p^2. Thus $F(p)$ takes the general form

$$F(p) = \int_0^\infty dm^2 \frac{\rho(m^2)}{p^2 - m^2 + i\epsilon} + f_0 + f_1 p^2 + \ldots, \tag{36}$$

where

$$\rho(m^2) = (2\pi)^3 \sum_{n\neq 0} |\langle 0|\, \pi^a_i(0)B^a_i(0)\, |n\rangle|^2 \delta(q - p_n)\Big|_{q^2=m^2, q^0\geq 0} \tag{37}$$

and $|n\rangle$ represents a physical state. Then we obtain

$$\varepsilon''(0) = \left(\frac{g^2}{8\pi^2}\right)^2 \left[\langle 0|\, B^a_i(0)^2 - \pi^a_i(0)^2 + f_0\, |0\rangle - \int dm^2 \frac{\rho(m^2)}{m^2}\right], \tag{38}$$

for the sum for θ-dependence in QCD.

The determination of the f_l is non-trivial. We only present some plausibility arguments regarding their general form. Let us define

$$Q = \frac{g^2}{32\pi^2} G^a_{\mu\nu}\tilde{G}^{a\mu\nu} = -\frac{\alpha}{2\pi}\pi^a_i B^a_i\,; \qquad \alpha = \frac{g^2}{4\pi}, \tag{39}$$

where we took $\theta = 0$. We assume that the singularity of $\mathrm{T}Q(x)Q(0)$ at $x = 0$ is determined by the short distance behavior of operator product $Q(x)Q(0)$ at space-like separations, and we consider the operator product expansion of this quantity. Note that Q is a renormalization group invariant dimension four operator. The possible leading nontrivial term in the expansion is

$$\int d^4x\, e^{ip\cdot x}\langle 0|\, Q(x)Q(0)\, |0\rangle \sim iA\langle 0|\, \alpha G^a_{\mu\nu}G^{a\mu\nu}\, |0\rangle \tag{40}$$

where we have used the renormalization group invariance of $\alpha G^a_{\mu\nu}G^{a\mu\nu}$; the factor of i comes from the transition to the Euclidean region. This term

generates a term independent of p^2 in $F(p)$. The other terms in the operator product expansion contain higher dimensional operators and are expected to vanish as $p^2 \to -\infty$ [2]. These arguments suggest that f_0 will be proportional to $\langle 0| \alpha G^a_{\mu\nu} G^{a\mu\nu} |0\rangle$ and $f_l = 0$ for $l \geq 1$. With the above assumptions we obtain

$$\varepsilon''(0) = f(\alpha)\langle 0| \alpha G^a_{\mu\nu} G^{a\,\mu\nu} |0\rangle - \frac{\alpha^2}{4\pi^2} \int dm^2 \frac{\rho(m^2)}{m^2}, \tag{41}$$

where $f(\alpha) = A + \alpha/(8\pi^2)$.

Let us turn to the possible modification of the sum rule by the inclusion of quark effects. It is known for QED triangle quark loop effect changes the naive canonical commutation relations for fermion currents but the commutator for gauge fields remain intact [10, 11, 12]. Thus we expect the canonical structure of π^a_i and G^a_i, especially their canonical commutation relations remain valid also when quarks are introduced. (In this case θ must be identified with the coefficient of $\tilde{G}G$ when the quark mass matrix is real and diagonal [2, 13].) The presence of quark loops will not alter the forms of (38) or (41), but will modify the explicit expressions for ρ and f_0 and $f(\alpha)$. In the presence of quarks the anomaly equation can be used to evaluate $\varepsilon''(0)$ in terms of fermionic operators; several publications [14, 15] have addressed this issue. These references, however, have apparently ignored the non-canonical quark current commutators implied by the anomaly. We will return to this issue in a future publication.

It is interesting to compare Eq. (38) with the interacting instanton gas result [16]. We get *positive* value for the first term:

$$\left(\frac{g^2}{8\pi^2}\right)^2 \left[\langle 0| B^a_i(0)^2 - \pi^a_i(0)^2 + f_0 |0\rangle\right] = 2\xi > 0, \tag{42}$$

where ξ is the instanton density. The θ-dependence of QCD (up order θ^2) is then determined by a competition between the (positive) first term and the

[2] We assume that the corresponding anomalous dimensions are not so large so as to invalidate this statement.

negative definite second term in (38). This raises the possibility of a cancellation, but a meaningful discussion of this possibility, as well as any other phenomenological implication, requires the introduction of quark effects.

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