Can the Feynman-Hellmann theorem be used to separate the connected- and disconnected-diagram contributions to the nucleon sigma term?

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Abstract

In recent lattice QCD studies, the Feynman-Hellmann theorem is often used to estimate separate contributions of the connected and disconnected diagrams to the nucleon sigma term. We demonstrate through a simple analysis within an effective model of QCD why this could be dangerous although the theorem is naturally expected to hold for the sum of the two contributions, i.e. the net nucleon sigma term.
I. INTRODUCTION

The nucleon sigma term $\Sigma_{\pi N}$ is believed to be a quantity of fundamental importance in that it gives a measure of the explicit chiral symmetry breaking of QCD. In fact, it characterizes the effect of finite quark mass on the mass of the nucleon as $M_N = M_0 + \Sigma_{\pi N}$, with $M_0$ being the nucleon mass in the chiral limit. Recently, the JLQCD collaboration reported an estimate of the nucleon sigma term with good precision based on the the overlap fermion action, which preserves exact chiral symmetry and flavor symmetries on the lattice [1]. They estimated the separate contributions of the connected and disconnected diagrams to the nucleon sigma term by utilizing the Feynman-Hellmann theorem derived within the framework of the partially quenched QCD (PQQCD), where the quarks that couple to external sources for the asymptotic hadrons, i.e. the valence quarks, are distinguished from those that contribute to the quark determinant, i.e. the sea quarks. They found that the connected diagram gives a dominant contribution to the nucleon sigma term and the disconnected-diagram contribution to it is fairly small. It appears to contradict our experience within the chiral quark soliton model (CQSM), in which we found the dominance of the Dirac-sea quarks over the valence quarks in this special observable [2]–[8]. (From the physical ground, the valence and Dirac-sea contributions in the CQSM is expected to correspond to the connected- and disconnected-diagram contributions in the lattice QCD, at least approximately.)

What is the cause of this discrepancy? There appears to be little reason to suspect the validity of the Feynman-Hellmann theorem, especially because it can be proved on quite general theoretical postulates. At the same time, however, one should recognize the fact that the general proof of the theorem in textbooks of quantum mechanics is given only for the total mass or the total Hamiltonian. (See [9], for instance.) If one divides the total contribution into two parts, it is highly nontrivial whether the theorem holds for the individual pieces separately. One might think that it is not a serious problem, since the Feynman-Hellmann theorem is anyhow expected to hold for the net nucleon sigma term and since only the sum is a quantity of physical interest. However, the authors of [1] made a semi-quenched estimate of the strange quark content of the nucleon within the same framework of two-flavor QCD utilizing the Feynman-Hellmann theorem, thereby being led to a remarkable conclusion that the $s\bar{s}$ components in the nucleon is very small in contrast with several past
estimates in the lattice QCD [10]-[12]. Whether this estimate is justified or not may depend on whether the use of the Feynman-Hellmann theorem for separating the connected- and disconnected-diagram contributions to the nucleon sigma term is justified or not.

The purpose of the present paper is to show why a naive application of the Feynman-Hellmann theorem can be dangerous when it is used for the separation of the nucleon sigma term into the two pieces. The strategy for verifying our claim is as follows. First, we recall the fact that, within the framework of the CQSM, we can directly calculate the separate contributions of the valence and Dirac-sea quarks to the nucleon sigma term, thereby confirming that the latter is dominant over the former. Second, we show that a naive application of the Feynman-Hellmann theorem leads to a totally different answer from the direct calculation, although the sum of the valence and Dirac-sea contributions are exactly the same in the two ways of calculating the nucleon sigma term. Next, we shall show that careful inspection of the derivation of the theorem indicates the necessity of a correction term, which fills up the gap between the direct calculation and the naive application of the Feynman-Hellmann theorem. Finally, bearing in mind our finding in the CQSM analysis, we shall make some remarks on the corresponding analysis of the nucleon sigma term in the lattice QCD by using the Feynman-Hellmann theorem.

II. THE NUCLEON SIGMA TERM IN THE CHIRAL QUARK SOLITON MODEL

A. A direct calculation

We begin with the effective Lagrangian of the chiral quark soliton model (CQSM) with an explicit chiral symmetry breaking [2],[3] :

\[ \mathcal{L} = \mathcal{L}_0 + \mathcal{L}', \]  

(1)

where \( \mathcal{L}_0 \) denotes the chiral symmetric part given by

\[ \mathcal{L}_0 = \bar{\psi}(x) \left[ i \gamma^5 \partial - M U^\gamma_5(x) \right] \psi(x), \]  

(2)

with \( M \) being the dynamically generated quark mass, and

\[ U^\gamma_5(x) = e^{i \gamma_5 \tau \cdot \pi(x)/f}. \]  

(3)
On the other hand,

\[ \mathcal{L}' = -m_0 \bar{\psi}(x) \psi(x), \]

is thought to simulate a small deviation from the chiral symmetry limit with \( m_0 \) being the bare quark mass. Note that the effective quark mass in the physical vacuum \( (U = 1) \) is given by \( \bar{M} = M + m_0 \). The model contains the parameters, \( M, m_0, f_\pi \) and some physical cutoffs. Throughout the present study, we set \( f_\pi = 93 \) MeV and \( M = 375 \) MeV, while the bare quark mass \( m_0 \) is varied around the reference value \( m_0 = 6 \) MeV. To fix the regularization parameters, we first define the effective action \( S_{\text{eff}}[U] \) through the relation

\[ Z = \int \mathcal{D}\pi \mathcal{D}\psi \mathcal{D}\psi^\dagger e^{i \int d^4x \mathcal{L}} = \int \mathcal{D}\pi e^{i S_{\text{eff}}[U]}. \]  

Next, to get rid of ultraviolet divergences contained in this definition, we introduce the regularized effective action in the proper-time regularization scheme by

\[ S_{\text{reg eff}}[U] = \frac{1}{2} i N_c \int_0^\infty \frac{d\tau}{\tau} \varphi(\tau) \text{Sp} \left( e^{-\tau D^\dagger D} - e^{-\tau D_0^\dagger D_0} \right), \]

with

\[ D = i \partial - MU^\gamma_5 - m_0, \quad D_0 = i \partial - (M + m_0). \]

The regularization function \( \varphi(\tau) \) is introduced so as to cut off divergences appearing as a singularity at \( \tau = 0 \). For determining it, we require that the regularized theory reproduce the correct normalization of the pion kinetic term as well as the mass term. Using the standard derivative-expansion technique, this gives two conditions:

\[ \frac{N_c M^2}{4 \pi^2} \int_0^\infty \frac{d\tau}{\tau} \varphi(\tau) e^{-\tau M^2} = f_\pi^2, \]

\[ m_0 \cdot \frac{N_c M}{2 \pi^2 f_\pi^2} \int_0^\infty \frac{d\tau}{\tau^2} \varphi(\tau) e^{-\tau M^2} = m_\pi^2. \]

Since Schwinger’s original choice \( \varphi(\tau) = \theta(\tau - 1/\Lambda^2) \), with \( \Lambda \) being a physical cutoff energy, cannot satisfy the above two conditions simultaneously, we use a slightly more complicated form as \[ 13, 14 \] \( \varphi(\tau) = c \theta \left( \tau - 1 / \Lambda_1^2 \right) + (1 - c) \theta \left( \tau - 1 / \Lambda_2^2 \right) \]

with \( c = 0.720, \Lambda_1 = 412.79 \) MeV and \( \Lambda_2 = 1330.60 \) MeV. The soliton construction in the CQSM starts with a static mean-field configuration of hedgehog shape as \[ 14, 15 \]

\[ U_0^\gamma_5(x) = e^{i \gamma_5 \cdot \mathbf{T} F(r)}. \]
The quark field in this mean-field obeys the Dirac equation:

$$H |n\rangle = E_n |n\rangle, \quad (12)$$

with

$$H = \frac{\alpha \cdot \nabla_i}{i} + M \beta e^{i \gamma_5 \tau \cdot \hat{r} F(r)} + m_0 \beta. \quad (13)$$

A characteristic feature of this Dirac equation is that one deep (single-quark) bound state appears from the positive-energy Dirac continuum. We call it the valence quark orbital. An object with baryon number one with respect to the physical vacuum is obtained by putting $N_c (= 3)$ quarks into this valence orbital as well as all the negative-energy (Dirac-sea) orbitals. Accordingly, the total energy of this baryon-number-one system is given by

$$E_{\text{static}}[U] = E_{\text{val}}[U] + E_{\text{sea}}[U]. \quad (14)$$

Here $E_{\text{val}}$ represents the valence quark contribution to the static energy, i.e.

$$E_{\text{val}}[U] = N_c E_0[U], \quad (15)$$

with $E_0$ being the eigen-energy of the valence quark level. On the other hand, $E_{\text{sea}}$ stands for the energy of the polarized Dirac sea. Regularizing it in the proper-time scheme, we have

$$E_{\text{sea}}[U] = \frac{N_c}{2} \frac{1}{\sqrt{4\pi}} \int_0^\infty \frac{d\tau}{\tau \sqrt{\tau}} \varphi(\tau) \left[ \sum_n e^{-\tau E_n^2} - \sum_k e^{-\tau \epsilon_k^2} \right]. \quad (16)$$
The energy of the physical vacuum \((U = 1)\) is subtracted here with \(\epsilon_k\) being the eigen-energy of the vacuum Hamiltonian \(H_0 \equiv H[U \to 1]\). The most probable pion-field configuration (or the self-consistent mean field) is determined by requiring the stationary condition for the total energy,

\[
\frac{\delta}{\delta F(r)} E_{\text{static}}[F(r)] = 0. \tag{17}
\]

This Hartree problem with infinitely many Dirac-sea orbital can be solved by using the numerical method of Kahana, Ripka and Soni \([16],[17]\). It also enables us to evaluate any nucleon observables with full inclusion of the Dirac-sea quarks. Of our particular interest here is the nucleon sigma term, which is defined as a \(\sum_{\pi N} = m_0 \tilde{\sigma}\) with \(m_0\) being the current quark mass and \(\tilde{\sigma}\) being the nucleon scalar charge given as \(\tilde{\sigma} = \langle N|\bar{u}u + \bar{d}d|N\rangle\). By taking care of the consistency with the basic equation of motion of the model, the regularized expression for the nucleon scalar charge \(\tilde{\sigma}\) is given as

\[
\tilde{\sigma} = \tilde{\sigma}_{\text{val}} + \tilde{\sigma}_{\text{sea}}, \tag{18}
\]

where

\[
\tilde{\sigma}_{\text{val}} = N_c \langle 0|\sigma^0|0\rangle, \tag{19}
\]

\[
\tilde{\sigma}_{\text{sea}} = -\frac{N_c}{2} \sum_n \mathcal{F}(E_n) \langle n|\sigma^0|n\rangle - \text{(vacuum subtraction)}, \tag{20}
\]

with the regularization function,

\[
\mathcal{F}(E_n) = \frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{d\tau}{\sqrt{\tau}} \varphi(\tau) E_n e^{-E_n^2 \tau}. \tag{21}
\]

Numerically, we find that

\[
\tilde{\sigma} \simeq 6.86, \tag{22}
\]

with

\[
\tilde{\sigma}_{\text{val}} \simeq 1.91, \quad \tilde{\sigma}_{\text{sea}} \simeq 4.95, \tag{23}
\]

which clearly show the dominance of the Dirac-sea contribution over the valence quark one. (With the choice \(m_0 = 6\) MeV, the above nucleon scalar charge gives \(\sum_{\pi N} \simeq 41.2\) MeV. We recall that the nucleon scalar charge, especially its Dirac-sea contribution, is a quantity which is extremely sensitive to the regularization scheme. The Pauli-Villars regularization scheme, which is also used frequently in the CQSM, leads to much larger nucleon sigma term ranging from 48 MeV to 72 MeV depending on the bare quark mass \(m_0\) \([4],[8]\).) Anyhow,
the predictions of the CQSM shown above appears to be qualitatively consistent with the results of the older simulations in quenched lattice QCD by based on the Wilson quark action [10]-[12]. (These old calculations by using the Wilson-type fermion, which violate the chiral symmetry on the lattice, were criticized, however. The criticism is that such calculations can give rise to a significant lattice artifacts in the sea quark content arising from the sea quark mass dependence of the additive mass renormalization and lattice spacing [19],[1].) It however appears to contradict the recent results of JLQCD collaborations by utilizing the Feynman-Hellmann theorem within the framework of the overlap fermion, which indicates the dominance of the contribution of the connected diagram over that of the disconnected one [1]. What is the cause of this discrepancy? To answer this question, we think it useful to evaluate the nucleon scalar charge by utilizing the Feynman-Hellmann theorem within the same CQSM.

B. A naive application of the Feynman-Hellmann theorem

We begin with the general statement of the Feynman-Hellmann theorem. The theorem states that

$$\frac{\partial}{\partial \alpha} E = \langle \Psi(\alpha) | \frac{\partial H(\alpha)}{\partial \alpha} | \Psi(\alpha) \rangle,$$  

(24)

where

- $H(\alpha)$ is a Hamiltonian operator depending on a continuous parameter $\alpha$.
- $| \Psi(\alpha) \rangle$ is an eigenstate of the Hamiltonian, depending implicitly upon $\alpha$.
- $E$ is the eigen-energy of the Hamiltonian $H(\alpha)$.

In our present application, the bare quark mass $m_0$ plays the role of the parameter $\alpha$, and the Hamiltonian is given by

$$H(m_0) = \frac{\alpha \cdot \nabla}{i} + M \beta e^{i\gamma} \tau_i \hat{r}_i F(r) + m_0 \beta.$$  

(25)

Thus, we obtain

$$\frac{\partial H}{\partial m_0} = \beta = \gamma^0.$$  

(26)

On the other hand, the eigenstate are given as

$$| \Psi(m_0) \rangle = \prod_{n \in \text{occ}} a_n^\dagger | \text{vac} \rangle,$$  

(27)
where \( a_n^\dagger \) represents the creation operator that creates a quark in the single-quark eigenstate \(|n\rangle\) of the Hamiltonian \( H(m_0) \), while \(|\text{vac}\rangle\) is the corresponding empty vacuum. The Feynman-Hellmann theorem then dictates that

\[
\frac{\partial}{\partial m_0} E(m_0) = \langle \Psi(m_0) | \gamma^0 | \Psi(m_0) \rangle.
\]  

(28)

Since the r.h.s. is nothing but the scalar charge \( \bar{\sigma} \) of the nucleon, we immediately get

\[
\bar{\sigma} = \frac{\partial}{\partial m_0} E(m_0),
\]  

(29)

which is the anticipated result. Remembering that the total energy is given as the sum of the energy of the valence quarks and that of the Dirac-sea quarks, one would further expect that

\[
\bar{\sigma} = \bar{\sigma}_{\text{val}} + \bar{\sigma}_{\text{sea}},
\]  

(30)

with

\[
\bar{\sigma}_{\text{val}} = \frac{\partial}{\partial m_0} E_{\text{val}}(m_0),
\]  

(31)

\[
\bar{\sigma}_{\text{sea}} = \frac{\partial}{\partial m_0} E_{\text{sea}}(m_0).
\]  

(32)

Within the CQSM, we can solve the eigenvalue problem for any value of \( m_0 \) to obtain \( E_{\text{val}} \) and \( E_{\text{sea}} \) as functions of \( m_0 \), so that we can readily calculate the r.h.s. of (31) and (32). (The mean field, or the soliton profile function \( F(r) \), is fixed throughout this calculation.) In that way, we obtain

\[
\bar{\sigma} \simeq 6.87,
\]  

(33)

with

\[
\bar{\sigma}_{\text{val}} \simeq 11.18, \quad \bar{\sigma}_{\text{sea}} = -4.31.
\]  

(34)

This should be compared with the answer of the direct calculation of the nucleon scalar charge described in the previous subsection :

\[
\bar{\sigma}^{(D)} = \bar{\sigma}_{\text{val}}^{(D)} + \bar{\sigma}_{\text{sea}}^{(D)} \simeq 1.91 + 4.95 \simeq 6.86.
\]  

(35)

One finds that the two ways of calculating the nucleon scalar charge give totally different answers for the individual contributions of the valence and Dirac-sea quarks. Nevertheless, both give practically the same answer for the sum of the two contributions, i.e. for the
net scalar charge of the nucleon, or equivalently for the net nucleon sigma term. Roughly speaking, the valence and Dirac-sea contributions in the CQSM corresponds to the connected and disconnected-diagram contributions in the lattice QCD. Then, what should be clarified is the reason why the naive application of the Feynman-Hellmann theorem does not reproduce a correct answer for the individual contributions of the valence and Dirac-sea quarks to the nucleon scalar charge, even though the net result, i.e. the sum of them, is correctly reproduced.

C. A careful treatment and a resolution of the puzzle

To reveal the origin of the discrepancy above, we first recall a general proof of the Feynman-Hellmann theorem in the form convenient for our discussion below. We start with the expression of the energy given as

\[ E(\alpha) = \langle \Psi(\alpha) | H(\alpha) | \Psi(\alpha) \rangle. \]  

(36)

Here, we assume that \( |\Psi(\alpha)\rangle \) is normalized as \( \langle \Psi(\alpha) | \Psi(\alpha) \rangle = 1 \). For the proof of the theorem, the state \( |\Psi(\alpha)\rangle \) need not be an exact eigenstate of the Hamiltonian \( H(\alpha) \). For instance, it can be an approximate eigenstate in Hatree-Fock theory, which is variationally optimized with respect to the Hamiltonian \[9\]. Under a small variation of a parameter \( \alpha \), the change of \( E(\alpha) \) is given by

\[ \delta E(\alpha) = \langle \Psi(\alpha) | \delta H(\alpha) | \Psi(\alpha) \rangle \]

\[ + \langle \Psi(\alpha) | H(\alpha) | \delta \Psi(\alpha) \rangle + \langle \delta \Psi(\alpha) | H(\alpha) | \Psi(\alpha) \rangle. \]  

(37)

If the state \( |\Psi(\alpha)\rangle \) is variationaly optimized with respect to the Hamiltonian, the 2nd line of the above equation is expected to vanish, i.e.

\[ \langle \Psi(\alpha) | H(\alpha) | \delta \Psi(\alpha) \rangle + \text{c.c.} = 0, \]  

(38)

where, c.c. means the complex conjugate of the 1st term. We therefore obtain

\[ \delta E(\alpha) = \langle \Psi(\alpha) | \delta H(\alpha) | \Psi(\alpha) \rangle, \]  

(39)

or equivalently

\[ \frac{\partial}{\partial \alpha} E(\alpha) = \langle \Psi(\alpha) | \frac{\partial}{\partial \alpha} H(\alpha) | \Psi(\alpha) \rangle, \]  

(40)
which proves the celebrated Feynman-Hellmann theorem.

What happens if the Hamiltonian consists of two terms as

\[ H(\alpha) = H_1(\alpha) + H_2(\alpha). \]  

Here, we are imagining the decomposition of the total energy into the contribution of the valence quarks and that of the Dirac-sea quarks in the CQSM. Note that, in the CQSM, this decomposition can in fact be realized as follows:

\[ H_1 = \langle 0 | H | 0 \rangle a_0^\dagger a_0, \]
\[ H_2 = \sum_{n \neq 0} \langle n | H | n \rangle a_n^\dagger a_n, \]

by taking the eigenstates of the Dirac Hamiltonian \((25)\) as a complete set. Now, the change of \(E(\alpha)\) under the variation \(\alpha \to \alpha + \delta \alpha\) is given as

\[ \delta E(\alpha) = \delta E_1(\alpha) + \delta E_2(\alpha) = \langle \Psi(\alpha) | \delta H_1(\alpha) + \delta H_2(\alpha) | \Psi(\alpha) \rangle + \langle \Psi(\alpha) | H_1(\alpha) + H_2(\alpha) | \delta \Psi(\alpha) \rangle + \text{c.c.} \]

Assuming that \(|\Psi(\alpha)\rangle\) is variationally optimized with respect to the total Hamiltonian, it still holds that

\[ \langle \Psi(\alpha) | H_1(\alpha) + H_2(\alpha) | \delta \Psi(\alpha) \rangle + \text{c.c.} = 0. \]

However, this does not necessarily mean that \(H_1\) term and \(H_2\) term separately vanish as

\[ \langle \Psi(\alpha) | H_1(\alpha) | \delta \Psi(\alpha) \rangle + \text{c.c.} = 0, \]
\[ \langle \Psi(\alpha) | H_2(\alpha) | \delta \Psi(\alpha) \rangle + \text{c.c.} = 0. \]

What is meant by (45) is only the identity:

\[ \langle \Psi(\alpha) | H_1(\alpha) | \delta \Psi(\alpha) \rangle + \text{c.c.} = - \left[ \langle \Psi(\alpha) | H_2(\alpha) | \delta \Psi(\alpha) \rangle + \text{c.c.} \right]. \]

On account of this observation, we therefore propose a decomposition,

\[ \langle \Psi(\alpha) | \frac{\partial H_1(\alpha)}{\partial \alpha} | \Psi(\alpha) \rangle = \frac{\partial}{\partial \alpha} E_1(\alpha) - \left[ \langle \Psi(\alpha) | H_1(\alpha) | \frac{\partial \Psi(\alpha)}{\partial \alpha} \rangle + \text{c.c.} \right], \]
\[ \langle \Psi(\alpha) | \frac{\partial H_2(\alpha)}{\partial \alpha} | \Psi(\alpha) \rangle = \frac{\partial}{\partial \alpha} E_2(\alpha) - \left[ \langle \Psi(\alpha) | H_2(\alpha) | \frac{\partial \Psi(\alpha)}{\partial \alpha} \rangle + \text{c.c.} \right]. \]
Applying this result of general consideration to our case of interest, we obtain

\[ \bar{\sigma} = \bar{\sigma}_{\text{val}} + \bar{\sigma}_{\text{sea}}, \]  

(51)

with

\[ \bar{\sigma}_{\text{val}} = \bar{\sigma}^{(FH)}_{\text{val}} + \delta\bar{\sigma}_{\text{val}}, \]  

(52)

\[ \bar{\sigma}_{\text{sea}} = \bar{\sigma}^{(FH)}_{\text{sea}} + \delta\bar{\sigma}_{\text{sea}}. \]  

(53)

Here, the \( \bar{\sigma}^{(FH)} \) terms correspond to the answer obtained with naive application of the Feynman-Hellman theorem as explained in the subsection A, i.e.

\[ \bar{\sigma}^{(FH)}_{\text{val}} = \frac{\partial}{\partial m} E_{\text{val}}(m_0), \]  

(54)

\[ \bar{\sigma}^{(FH)}_{\text{sea}} = \frac{\partial}{\partial m} E_{\text{sea}}(m_0). \]  

(55)

On the other hand, the correction terms to this naive answer is given by

\[ \delta\bar{\sigma}_{\text{val}} = - \lim_{\Delta m_0 \to 0} \frac{\langle \Psi(m_0 + \Delta m_0) | H | \Psi(m_0 + \Delta m_0) \rangle^{\text{val}}}{\Delta m_0} - \frac{\langle \Psi(m_0) | H | \Psi(m_0) \rangle^{\text{val}}}{\Delta m_0}, \]  

(56)

\[ \delta\bar{\sigma}_{\text{sea}} = - \lim_{\Delta m_0 \to 0} \frac{\langle \Psi(m_0 + \Delta m_0) | H | \Psi(m_0 + \Delta m_0) \rangle^{\text{sea}}}{\Delta m_0} - \frac{\langle \Psi(m_0) | H | \Psi(m_0) \rangle^{\text{sea}}}{\Delta m_0}, \]  

(57)

with the simplified notation \( H = H(m_0) \). We emphasize that the identity (58) dictates that \( \delta\bar{\sigma}_{\text{val}} \) and \( \delta\bar{\sigma}_{\text{sea}} \) are not independent but must satisfy the constraint:

\[ \delta\bar{\sigma}_{\text{val}} + \delta\bar{\sigma}_{\text{sea}} = 0. \]  

(58)

That is, the above correction terms generally contribute to both of the valence quark term and the Dirac-sea term, but they are expected to cancel in the sum, i.e. in the net contribution to the nucleon scalar charge, or equivalently in the nucleon sigma term.

Since all the quantities appearing in the above discussion can be calculated explicitly within the CQSM, we can verify whether our theoretical consideration is correct or not. Shown in table I are the results of our numerical calculation for the relevant quantities. The 2nd row of the table show the contributions of the valence and Dirac-sea quarks to the quantity \( \bar{\sigma}^{(FH)} \) together with the sum of them, while the 3rd row give the corresponding contributions of correction term \( \delta\bar{\sigma} \). One sees that the valence quark contribution to \( \delta\bar{\sigma} \) is large and negative but the Dirac-sea contribution to \( \delta\bar{\sigma} \) has just the same magnitude with
TABLE I: The CQSM predictions for the nucleon scalar charge. The calculation by using the Feynman-Hellmann theorem is compared with the direct calculation.

|                | valence | Dirac-sea | total |
|----------------|---------|-----------|-------|
| $\bar{\sigma}^{(FH)}$ | 11.18   | - 4.31    | 6.87  |
| $\delta\bar{\sigma}$    | - 9.27  | 9.25      | - 0.02|
| $\bar{\sigma}^{(FH)} + \delta\bar{\sigma}$ | 1.91    | 4.94      | 6.85  |
| $\bar{\sigma}^{(D)}$    | 1.91    | 4.95      | 6.86  |

opposite sign (aside from very small numerical error). The 3rd row represents the sum of $\bar{\sigma}^{(FH)}$ term and $\delta\bar{\sigma}$ term, whereas the 4th row stands for the answer of the direct calculation of the nucleon scalar charge. One can clearly convince that, if one properly takes account of the correction term $\delta\bar{\sigma}$ in addition to the term $\bar{\sigma}^{(FH)}$ naively expected from the Feynman-Hellmann theorem, the answers of the direct calculation is legitimately reproduced not only for the net scalar charge but also for the individual contributions of the valence and of the Dirac-sea quarks.

Now, we have confirmed that, within the framework of the CQSM, the direct calculation and the indirect calculation by utilizing the (slightly modified) Feynman-Hellmann theorem give exactly the same answer for the decomposition of the valence and Dirac-sea contributions to the nucleon sigma term. The answer clearly shows the dominance of the contribution of the Dirac-sea quarks over that of the valence quarks, in sharp contrast to the corresponding answer of the lattice QCD simulation with use of the Feynman-Hellmann theorem [1]. The lattice QCD version of the Feynman-Hellmann theorem is derived based on the framework of partially quenched QCD (PQQCD) [1],[18], where the valence quarks that coupled to external sources for the asymptotic hadrons are distinguished from the sea quarks that contribute to the quark determinant [20],[21]. By treating the masses of the valence and sea quarks as independent variables, the PQQCD version of Feynman-Hellmann theorem is written down in the following form :

$$\frac{\partial M_N}{\partial m_{val}} = \langle N | \bar{u} u + \bar{d} d | N \rangle_{\text{conn}}, \quad (59)$$
\[ \frac{\partial M_N}{\partial m_{\text{sea}}} = \langle N | \bar{u} u + \bar{d} d | N \rangle_{\text{disc}}, \quad (60) \]

where the short-hand notation to omit the vacuum subtraction term \(-V \langle 0 | \bar{u} u + \bar{d} d | 0 \rangle\) is used for the disconnected piece. A general strategy for evaluating these terms are as follows. One first generates statistically independent ensembles of gauge field configurations at several different sea quarks masses. After that, one measures the nucleon mass for various valence quark masses on each of those gauge ensembles. This in principle makes it possible to evaluate valence and sea quark mass dependence of the nucleon mass. The physical answer for the nucleon sigma term is then obtained by calculating the derivatives (59) and (60) of \( M_N \) at the unitary point \( m_{\text{sea}} = m_{\text{val}} \). (In practice, the simulation in the chiral region is not economical, so that the results of simulations in the larger quark mass region are extrapolated to obtain answers corresponding to the chiral region with the help of the partially quenched baryon chiral perturbation theory [22].)

It appears that there is no question about this general prescription. How can we reconcile the prediction of the lattice QCD with that of the CQSM, then? Naturally, an easy explanation is to claim that the decomposition of the valence and Dirac-sea contributions to the nucleon sigma term in the CQSM does not simply correspond to that of the connected and disconnected contributions to the same quantity in the lattice QCD. We cannot deny this possibility completely, because there is no rigorous correspondence between the two theories and their decompositions of the nucleon sigma term. From a physical viewpoint, however, the discrepancy seems too large (or more than quantitative) to accept this naive conclusion. In our opinion, this discrepancy should be taken more seriously. If there is any resolution to this problem, we conjecture that it must be traced back to a difference between the treatment of the valence and sea quarks in the CQSM and that in the partially quenched QCD. In our framework of the CQSM, we do not need to distinguish the masses of the valence and Dirac-sea quarks. They are treated on the equal footing from the beginning to the end. On the other hand, there is an apparent asymmetry in the treatment of the valence and sea quarks in the PQQCD. (We are talking about the asymmetry in the treatment of the valence and sea quarks when generating ensemble of gauge field configuration. Ideally, all the field configurations of the nucleon constituents, i.e. the gluon field, the valence and sea quarks, should be determined according to a self-consistent dynamics of QCD.) It may be certainly true that the masses of the valence and sea quarks are taken equal at the
end of calculation, and that the physical answers obtained in this unitary limit is taken to be physical [21]. This would also apply to the PQCD version of the Feynman-Hellmann theorem. In consideration of fundamental importance of the problem, however, we think it very important to check the validity of the Feynman-Hellmann theorem in an explicit manner by carrying out a direct calculation of the connected- and disconnected-diagram contributions to the nucleon sigma term within the same framework of the overlap fermion. (The direct calculation means a calculation of the three point functions with an insertion of the scalar density operators.)

Before ending this subsection, it may be useful to recall one plausible argument, which strongly indicates that the contribution of the valence quarks cannot be a dominant term of the nucleon sigma term [23]. As is well known, the recent analyses of the pion-nucleon scattering amplitude favor fairly large nucleon sigma term ranging from 50 MeV to 70 MeV [24]-[26]. Depending on the uncertainty of the average $u$- and $d$-quark masses, this implies fairly large nucleon scalar charge $\bar{\sigma}$ of the order of 10. As we shall argue below, it is unlikely that such a large value of $\bar{\sigma}$ can be explained by the contribution of three valence quarks alone. To convince it, let us consider a relativistic bound state of $N_c$ (= 3) quarks. Assume that these quarks are confined in some mean field or confining potential. A typical example is the famous MIT bag model. The ground state wave function of this popular model is given as

$$
\psi_{g.s.}(r) = \begin{pmatrix} f(r) \chi_s \\ i\sigma \cdot \hat{r} g(r) \chi_s \end{pmatrix},
$$

(61)

where $f(r)$ and $g(r)$ are the radial wave functions of the upper and lower components, while $\chi_s$ is an appropriate spin wave function. The nucleon scalar charge in this model is easily obtained as

$$
\bar{\sigma} = \langle N | \bar{u}u + \bar{d}d | N \rangle = N_c \int_0^R \left[ (f(r))^2 - (g(r))^2 \right] r^2 dr,
$$

(62)

with $R$ the bag radius. Undoubtedly, the magnitude of this quantity is smaller than $N_c$, since the radial functions satisfy the normalization,

$$
\int_0^R \left[ (f(r))^2 + (g(r))^2 \right] r^2 dr = 1.
$$

(63)

It is clear that this observation does not depend on the exact form of the mean field or the confining potential, so that it is quite general. As a consequence, for any model of the
nucleon, which contains $N_c$ valence quark degrees of freedom alone, we must conclude that there exists a upper bound such that

$$\bar{\sigma}_{\text{val}} < N_c.$$  \hfill (64)

Our prediction in the CQSM, i.e. $\bar{\sigma}_{\text{val}} \simeq 1.91$, as well as the direct calculation in the quenched lattice QCD in [10], i.e. $\langle N | \bar{u} u + \bar{d} d | N \rangle_{\text{connected}} \simeq 2.323(15)$, satisfy the above bound. On the other hand, the recent estimate by the JLQCD collaboration utilizing the Feynman-Hellmann theorem [1], i.e. $\langle N | \bar{u} u + \bar{d} d | N \rangle_{\text{connected}} \simeq 5.27(75) - 7.92(8)$, lies outside this bound. Again, highly desirable is a direct calculation of the nucleon sigma term within the framework of the overlap fermion, without utilizing the Feynman-Hellmann theorem.

III. SUMMARY AND CONCLUSION

In summary, we have investigated the nucleon sigma term or the nucleon scalar charge within a simple effective model of QCD, i.e. the chiral quark soliton model. It was demonstrated that the naive application of the Feynman-Hellmann theorem does not reproduce the correct answer for the separate contributions of the valence and Dirac-sea quarks to the nucleon sigma term, which can be obtained by the direct calculation within the same model. It was also shown that a careful inspection of the derivation of the Feynman-Hellmann theorem indicates the necessity of a correction term, which fills up the gap between the direct calculation and the naive application of the Feynman-Hellmann theorem. Anyhow, by using two completely independent methods of calculation, we have confirmed that the contribution of the Dirac-sea quarks dominates over that of the valence quarks in this unique observable of the nucleon.

This observation however appears to contradict the corresponding answer of the recent lattice QCD simulation by JLQCD collaboration based on the action of overlap fermion. They estimated the separate contributions of the connected and disconnected diagrams to the nucleon sigma term by utilizing the lattice QCD version of the Feynman-Hellmann theorem, which is derived within the scheme of PQQCD, and found that the connected diagram gives a dominant contribution to the nucleon sigma term and the disconnected-diagram contribution is of secondary importance. Although we do not have any convincing reasoning
to suspect the validity of the lattice QCD version of the Feynman-Hellmann theorem, it is highly desirable to check the validity of it by a direct calculation of the nucleon sigma term within the same framework of overlap fermion. This is especially so, because the separation of the nucleon sigma term into the contributions of valence and sea quarks seems to be a very delicate operation as our model analysis has shown, and also because the direct confirmation of the theorem is of fundamental importance to check whether the theoretical framework of the PQQCD, which was invented for handling loops of sea quarks in the lattice QCD, is working as it is expected.

Acknowledgments

We would like to thank Prof. T. Onogi for useful discussion about the Feynman-Hellmann theorem in lattice QCD. This work is supported in part by a Grant-in-Aid for Scientific Research for Ministry of Education, Culture, Sports, Science and Technology, Japan (No. C-21540268)

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