Spin and Orbital Angular Momentum in Gauge Theories: Nucleon Spin Structure and Multipole Radiation Revisited

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We address and solve the long-standing gauge-invariance problem of the nucleon spin structure. Explicitly gauge-invariant spin and orbital angular momentum operators of quarks and gluons are obtained. This was previously thought to be an impossible task and opens a more promising avenue towards the understanding of the nucleon spin. Our research also justifies the traditional use of the canonical, gauge-dependent angular momentum operators of photons and electrons in the multipole-radiation analysis and labeling of atomic states and sheds much light on the related energy-momentum problem in gauge theories, especially in connection with the nucleon momentum.

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The dilemma in separating the nucleon spin.—As a composite particle, the nucleon naturally obtains its spin from the spin and orbital motion of its constituents: quarks and gluons. From a theoretical point of view, the first task in studying the nucleon spin structure is to find out the appropriate operators for the spin and orbital angular momentum of the quark and gluon fields. Given these operators, one can then study their matrix elements in a polarized nucleon state and investigate how these matrix elements can be related to experimental measurements. Disturbingly and surprisingly, after 20 years of extensive discussions of the nucleon spin structure [1–5], this first task has never been done and has even largely eluded the attention of the community.

At first thought, it seems an elementary exercise to derive the quark and gluon angular momentum operators. From the Lagrangian $\mathcal{L} = -\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + \bar{\psi}(i\gamma^\mu \mathbb{D}_\mu - m)\psi$, where $\mathbb{D}_\mu = \partial_\mu + ig\mathbb{A}_\mu$ and $\mathbb{A}_\mu \equiv A^a_\mu T^a$ [with T^a the generators of the color SU(3) group], one can promptly follow Nöther's theorem to write down the canonical expression of the conserved QCD angular momentum

$$\vec{J}_{\rm QCD} = \int d^3x\psi^\dagger \frac{1}{2}\vec{\Sigma}\psi + \int d^3x\psi^\dagger \vec{x}\times\frac{1}{i}\vec{\nabla}\psi + \int d^3x\vec{E}^a \times \vec{A}^a + \int d^3x E^{ai}\vec{x}\times\vec{\nabla}A^{ai} \equiv \vec{S}_q + \vec{L}_q + \vec{S}_g + \vec{L}_g \quad (1)$$

and readily identify the four terms here as the quark spin [$\vec{\Sigma} = {\rm diag}(\vec{\sigma},\vec{\sigma})$ and $\vec{\Sigma}\times\vec{\Sigma} = i\vec{\Sigma}$], quark orbital angular momentum, gluon spin, and gluon orbital angular momentum, respectively. However, except for the quark spin, all of the other three terms are gauge-dependent and thus have obscure physical meanings. In this regard, it should be noted that the total angular momentum is nonetheless gauge-invariant (as it must be). This can be seen from an alternative, explicitly gauge-invariant expression [6,7]:

$$\vec{J}_{\rm QCD} = \int d^3x\psi^\dagger \frac{1}{2}\vec{\Sigma}\psi + \int d^3x\psi^\dagger \vec{x}\times\frac{1}{i}\vec{\mathbb{D}}\psi + \int d^3x\vec{x} \times (\vec{E}^a\times\vec{B}^a) \equiv \vec{S}_q + \vec{L}'_q + \vec{J}'_g. \quad (2)$$

This is obtained from Eq. (1) by adding a surface term

$$\int d^3x\vec{\nabla}\cdot[\vec{E}^a(\vec{A}^a\times\vec{x})], \quad (3)$$

which vanishes after integration. Since all of the terms in Eq. (2) are separately gauge-invariant, it may seem appropriate to identify $\vec{L}'_q$ as the quark orbital angular momentum and $\vec{J}'_g$ as the total gluon angular momentum. However, a further decomposition of $\vec{J}'_g$ into gauge-invariant gluon spin and orbital parts is lacking. Moreover, neither $\vec{L}'_q$ nor $\vec{J}'_g$ obeys the fundamental angular momentum algebra $\vec{J}\times\vec{J} = i\vec{J}$ (although $\vec{J}'_g$ does when the quark field is absent); hence, they cannot be the relevant rotation generators [7]. It has long been assumed by the community that the reconciliation of gauge invariance and the angular momentum algebra is not possible and that gauge-invariant, local gluon spin and orbital angular momentum operators do not exist [4].

The QED problem revisited.—Since QED is also a gauge theory, the problems above first emerged there. In fact, by simply dropping the color indices, Eqs. (1) and (2) become exactly the expressions for the electron and photon angular momenta, which we denote as

$$\vec{J}_{\rm QED} = \vec{S}_e + \vec{L}_e + \vec{S}_\gamma + \vec{L}_\gamma \quad (4)$$

$$= \vec{S}_e + \vec{L}'_e + \vec{J}'_\gamma. \quad (5)$$

Equation (5) is obtained from Eq. (4) by adding the same surface term as in (3) but without the color indices.

Similarly to the situation in QCD, neither Eq. (4) nor Eq. (5) is fully satisfactory: On the one hand, the canonical angular momentum operators in Eq. (4) are what people use familiarly in discussing polarized atomic states and radiation, but the gauge dependence of these operators leads to an uneasy concern about many calculations. As one example, the labeling of atomic states, which uses eigenvalues of the electron orbital angular momentum operator $\vec{L}_e = \int d^3x \psi^\dagger \vec{x} \times \frac{1}{i}\vec{\nabla}\psi$, seems gauge-dependent. For another example, the multipole-radiation analysis, which employs the multipole-field wave function constructed with photon spin and orbital angular momentum operators, seems again gauge-dependent. On the other hand, the gauge-invariant operators in Eq. (5) $\vec{L}'_e$ and $\vec{J}'_\gamma$ are not appropriate for constructing angular momentum eigenstates (because, as we remarked above, they are not angular momentum operators at all) and do not separate photon spin from photon orbital angular momentum. It is stated in common textbooks that gauge invariance prohibits the separation of photon angular momentum into spin and orbital contributions [8,9], yet both photon spin and orbital angular momentum have been measured separately by experiments [10–16].

Despite the gauge dependence of Eq. (4), all QED angular momentum calculations based on it seem to agree well with experiments. It is therefore hard to believe that all of those discussions, including the whole multipole-radiation analysis and labeling of atomic, nuclear, and hadronic states, are meaningless. Enlightened by earlier clarifications [17,18], we find that there exists indeed a satisfactory and decisive answer for the question of spin and orbital angular momentum in QED:

$$\begin{aligned}\vec{J}_{\rm QED} &= \int d^3x \psi^\dagger \frac{1}{2}\vec{\Sigma}\psi + \int d^3x \psi^\dagger \vec{x} \times \frac{1}{i}\vec{D}_{\rm pure}\psi \\ &\quad + \int d^3x \vec{E} \times \vec{A}_{\rm phys} + \int d^3x E^i \vec{x} \times \vec{\nabla} A^i_{\rm phys} \\ &\equiv \vec{S}_e + \vec{L}''_e + \vec{S}''_\gamma + \vec{L}''_\gamma. \end{aligned} \quad (6)$$

Here $\vec{D}_{\rm pure} \equiv \vec{\nabla} - ie\vec{A}_{\rm pure}$, $\vec{A}_{\rm pure} + \vec{A}_{\rm phys} \equiv \vec{A}$, and the two parts are defined via

$$\vec{\nabla} \cdot \vec{A}_{\rm phys} = 0, \quad (7)$$

$$\vec{\nabla} \times \vec{A}_{\rm pure} = \vec{0}. \quad (8)$$

These are nothing but the transverse and longitudinal components of the vector potential $\vec{A}$. The subscripts used here are intended to make the physical (vs. pure-gauge) content clear and to prepare for the generalization to QCD. With the boundary condition that $\vec{A}$, $\vec{A}_{\rm pure}$, and $\vec{A}_{\rm phys}$ all vanish at spatial infinity, Eqs. (7) and (8) prescribe a unique decomposition of $\vec{A}$ into $\vec{A}_{\rm pure}$ and $\vec{A}_{\rm phys}$ and dictate their distinct gauge transformation properties:

$$\vec{A}_{\rm pure} \rightarrow \vec{A}'_{\rm pure} = \vec{A}_{\rm pure} + \vec{\nabla}\Lambda, \quad (9)$$

$$\vec{A}_{\rm phys} \rightarrow \vec{A}'_{\rm phys} = \vec{A}_{\rm phys}, \quad (10)$$

under a gauge transformation Λ. Equations (8) and (9) tell us that, in QED, $\vec{A}_{\rm pure}$ is a pure-gauge field in all gauges and that it transforms in the same manner as does the full vector field: $\vec{A} \rightarrow \vec{A}' = \vec{A} + \vec{\nabla}\Lambda$. On the other hand, the transverse field $\vec{A}_{\rm phys}$ is unaffected by gauge transformations and so can be regarded as the "physical" part of $\vec{A}$.

Equation (6) is obtained from Eq. (4) by adding another surface term:

$$\int d^3x \vec{\nabla} \cdot [\vec{E}(\vec{A}_{\rm pure} \times \vec{x})]. \quad (11)$$

Now we have all of the elements needed to explain how Eq. (6) gives the correct expressions for the spin and orbital angular momenta of electrons and photons, including their densities. First of all, the total $\vec{J}_{\rm QED}$ given by Eq. (6) equals that in Eqs. (4) and (5), for they merely differ by surface terms. Second, the gauge transformation properties of $\vec{A}_{\rm pure}$ and $\vec{A}_{\rm phys}$ show that each *density* term in Eq. (6) is separately gauge-invariant (and, hence, so is the integrated operator). Third, like the canonical $\vec{L}_e$, the gauge-invariant $\vec{L}''_e$ satisfies the angular momentum algebra $\vec{J} \times \vec{J} = i\vec{J}$. This is due to the property of $\vec{A}_{\rm pure}$ in Eq. (8). Finally, we note that, in the Coulomb gauge, $\vec{\nabla} \cdot \vec{A} = 0$, so the longitudinal (pure-gauge) field $\vec{A}_{\rm pure}$ vanishes; thus, all quantities in Eq. (6) coincide with their canonical counterparts in Eq. (4). This observation is of vital importance. It reveals that the gauge-invariant quantities in Eq. (6) can all be conveniently computed via the canonical operators in the Coulomb gauge. This is actually what people (implicitly) do in studying atomic and electromagnetic angular momenta (such as in multipole radiation), including the recent measurements of the photon orbital angular momentum [11–16]. It is thus natural that these studies always obtain reasonable results.

Hindsight for QED and solution for QCD.—After confirming that Eq. (6) is indeed the correct and satisfactory answer for angular momenta in QED, we can observe something about it in hindsight. The form of Eq. (6) could have been guessed by reasonable physical considerations: The photon angular momentum should contain only the physical part of the gauge field, which should, nevertheless, not appear in the expression for the electron orbital angular momentum $\vec{L}''_e$. The latter should thus include only the nonphysical $\vec{A}_{\rm pure}$, so as to cancel the equally nonphysical phase dependence of the electron field, and keep the whole $\vec{L}''_e$ gauge-invariant. From this hindsight for QED, it is natural to expect that the correct, gauge-invariant expressions of QCD angular momenta should be

$$\vec{J}_{\rm QCD} = \int d^3x\psi^\dagger\frac{1}{2}\vec{\Sigma}\psi + \int d^3x\psi^\dagger\vec{x}\times\frac{1}{i}\vec{\mathbb{D}}_{\rm pure}\psi + \int d^3x\vec{E}^a \times\vec{A}^a_{\rm phys} + \int d^3xE^{ai}\vec{x}\times\vec{\nabla}A^{ai}_{\rm phys} \equiv \vec{S}_q + \vec{L}''_q + \vec{S}''_g + \vec{L}''_g, \tag{12}$$

where $\vec{\mathbb{D}}_{\rm pure} \equiv \vec{\nabla} - ig\vec{\mathbb{A}}_{\rm pure}$ and $\vec{\mathbb{A}}_{\rm pure} \equiv \vec{A}^a_{\rm pure}T^a$. The essential task remaining now is to properly define the pure-gauge field $\vec{\mathbb{A}}_{\rm pure}$ and the physical field $\vec{\mathbb{A}}_{\rm phys} \equiv \vec{A}^a_{\rm phys}T^a$ so that they have the desired gauge transformation properties and to prove that the sum of the four terms in Eq. (12) equals that in Eqs. (1) and (2). This, however, turns out to be nontrivial.

The parallel construction of Eqs. (7) and (8) obviously does not work in QCD. For one thing, $\vec{\mathbb{A}}_{\rm pure}$ defined by $\vec{\nabla}\times\vec{\mathbb{A}}_{\rm pure} = \vec{0}$ is not a pure-gauge term in QCD; for another, $\vec{\nabla}\cdot\vec{\mathbb{A}}_{\rm phys} = \vec{0}$ and $\vec{\nabla}\times\vec{\mathbb{A}}_{\rm pure} = \vec{0}$ are not invariant under the SU(3) gauge transformation:

$$\mathbb{A}_\mu \to \mathbb{A}'_\mu = U\mathbb{A}_\mu U^\dagger - \frac{i}{g}U\partial_\mu U^\dagger. \tag{13}$$

To make $\vec{\mathbb{A}}_{\rm pure}$ a pure-gauge term in QCD, we require, instead of Eq. (8), that

$$\vec{\mathbb{D}}_{\rm pure}\times\vec{\mathbb{A}}_{\rm pure} = \vec{\nabla}\times\vec{\mathbb{A}}_{\rm pure} - ig\vec{\mathbb{A}}_{\rm pure}\times\vec{\mathbb{A}}_{\rm pure} = \vec{0}. \tag{14}$$

This provides two independent equations for $\vec{\mathbb{A}}_{\rm pure}$. We still need a third equation that plays the same role as Eq. (7) does in QED, so that $\vec{\mathbb{A}}_{\rm phys}$ and $\vec{\mathbb{A}}_{\rm pure}$ have the required transformation properties:

$$\vec{\mathbb{A}}_{\rm pure} \to \vec{\mathbb{A}}'_{\rm pure} = U\vec{\mathbb{A}}_{\rm pure}U^\dagger + \frac{i}{g}U\vec{\nabla}U^\dagger, \tag{15}$$

$$\vec{\mathbb{A}}_{\rm phys} \to \vec{\mathbb{A}}'_{\rm phys} = U\vec{\mathbb{A}}_{\rm phys}U^\dagger. \tag{16}$$

To seek this third equation, we proceed inversely by applying these transformations to examine the gauge invariance of each operator in Eq. (12). The reason why this is possible will be clear shortly below.

The quark orbital angular momentum $\vec{L}''_q$ provides no further constraints. Equations (14) and (15) guarantee its gauge invariance, as well as the correct angular momentum algebra $\vec{L}''_q\times\vec{L}''_q = i\vec{L}''_q$. The gluon spin $\vec{S}''_g$ provides no further constraints either. Equation (16) tells us that it is gauge-invariant. However, the situation for the gluon orbital angular momentum $\vec{L}''_g$ is different. Unlike in QED, $\vec{\mathbb{A}}_{\rm phys}$ here is gauge-covariant instead of invariant, which leads to the gauge transformation of $\vec{L}''_g$:

$$\begin{aligned} E^{ai}\vec{x}\times\vec{\nabla}A^{ai}_{\rm phys} &= 2{\rm Tr}\{\mathbb{E}^i\vec{x}\times\vec{\nabla}\mathbb{A}^i_{\rm phys}\} \to 2{\rm Tr}\{U\mathbb{E}^iU^\dagger\vec{x} \times\vec{\nabla}(U\mathbb{A}^i_{\rm phys}U^\dagger)\} \\ &= 2{\rm Tr}\{\mathbb{E}^i\vec{x}\times\vec{\nabla}\mathbb{A}^i_{\rm phys}\} + 2{\rm Tr}\{\vec{x}\times U^\dagger(\vec{\nabla}U) \times(\vec{\mathbb{A}}_{\rm phys}\cdot\vec{\mathbb{E}} - \vec{\mathbb{E}}\cdot\vec{\mathbb{A}}_{\rm phys})\}, \end{aligned} \tag{17}$$

where $\vec{\mathbb{E}} \equiv \vec{E}^aT^a$. Hence, to make $\vec{L}''_g$ invariant under arbitrary gauge transformations, we have to set

$$[\vec{\mathbb{A}}_{\rm phys}, \vec{\mathbb{E}}] \equiv \vec{\mathbb{A}}_{\rm phys}\cdot\vec{\mathbb{E}} - \vec{\mathbb{E}}\cdot\vec{\mathbb{A}}_{\rm phys} = 0. \tag{18}$$

This is the third equation that we seek. The remaining task is to cross-check the consistency of whether or not Eqs. (14) and (18) dictate the transformation properties in Eqs. (15) and (16).

Before making this cross-check, we first make another vital check, namely, whether the definitions of $\vec{\mathbb{A}}_{\rm pure}$ and $\vec{\mathbb{A}}_{\rm phys}$ by Eqs. (14) and (18) ensure that the total angular momentum in Eq. (12) is to equal that in Eqs. (1) and (2). Since no more tricks are available, the answer must be positive, or our entire approach will founder. A slightly lengthy but straightforward calculation shows that the answer is indeed positive. With the definitions in Eqs. (14) and (18), Eq. (12) can be obtained from Eq. (1) by adding a surface term similar to (11) for QED:

$$\int d^3x\vec{\nabla}\cdot[\vec{E}^a(\vec{A}^a_{\rm pure}\times\vec{x})]. \tag{19}$$

As to the cross-check, we note that $\vec{\mathbb{A}}'_{\rm pure}$ and $\vec{\mathbb{A}}'_{\rm phys}$ given by Eqs. (15) and (16) are solutions of

$$\vec{\mathbb{D}}'_{\rm pure}\times\vec{\mathbb{A}}'_{\rm pure} = \vec{0}, \tag{20}$$

$$[\vec{\mathbb{A}}'_{\rm phys}, \vec{\mathbb{E}}'] = 0, \tag{21}$$

where $\vec{\mathbb{D}}'_{\rm pure} \equiv \vec{\nabla} - ig\vec{\mathbb{A}}'_{\rm pure}$ and $\vec{\mathbb{E}}' = U\vec{\mathbb{E}}U^\dagger$. The remaining question is whether Eqs. (20) and (21) have any other solution than that given by Eqs. (15) and (16). This is equivalent to asking whether Eqs. (14) and (18) uniquely determine the decomposition of $\vec{\mathbb{A}}$ into $\vec{\mathbb{A}}_{\rm pure}$ and $\vec{\mathbb{A}}_{\rm phys}$ or, essentially, whether the constraint $[\vec{\mathbb{A}}, \vec{\mathbb{E}}] = 0$ fixes the gauge completely. This is a tricky question, for, unlike in QED, many gauges in QCD suffer from topological complexity such as Gribov copies [19]. Fortunately, such complexity does not bother us here: If supplementary conditions are needed to restrict the solutions of Eqs. (20) and (21) to that given by Eqs. (15) and (16), they can simply be added, without affecting the equivalence of Eq. (12) with Eqs. (1) and (2) and without affecting the gauge invariance of the angular momentum operators we constructed, because these properties rely only on Eqs. (14)–(16) and (18).

Remarks and discussion.—(i) We have noted that, for QED in the Coulomb gauge $\vec{\nabla}\cdot\vec{A} = 0$, Eq. (6) coincides with Eq. (4). Similarly, for QCD, in the gauge $[\vec{\mathbb{A}}, \vec{\mathbb{E}}] = 0$ (together with possible supplementary conditions to completely fix the gauge), Eq. (12) coincides with Eq. (1). Namely, in actual calculations, QCD shares the same nice feature as in QED that the gauge-invariant, physically meaningful angular momenta can be conveniently computed via their canonical, gauge-dependent counterparts in a physical gauge in which the pure-gauge component vanishes. From the QCD equation of motion $\vec{\nabla}\cdot\vec{\mathbb{E}} = ig[\vec{\mathbb{A}}, \vec{\mathbb{E}}] + g\psi^\dagger T^a\psi T^a$, we see that the gauge $[\vec{\mathbb{A}}, \vec{\mathbb{E}}] = 0$ says essentially that the (gauge-dependent) color charge carried by gluons vanishes. So $[\vec{\mathbb{A}}, \vec{\mathbb{E}}] = 0$ has the sense of a ''generalized'' Coulomb gauge, for it leads to an equation of motion $\vec{\nabla}\cdot\vec{E}^a = g\psi^\dagger T^a\psi$, similar to Gauss' law in QED.

(ii) Our construction guarantees that all angular momentum operators transform properly under spatial translation and rotation. To figure out how they transform under boost, we need to carry out the canonical quantization procedure (preferably in the physical gauge in which the pure-gauge terms vanish) and compute the commutators of the angular momentum operators with the interaction-involving boost generators. This nontrivial task will be our next work.

(iii) In the literature, there have been various discussions about decomposing the Yang-Mills field into several components representing different degrees of freedom, based mainly on group-theoretical considerations [20–22]. It would be very interesting to investigate how these decompositions are related to ours, which is dictated by the requirement of a physically meaningful angular momentum expression.

(iv) The so-called gluon polarization ΔG being measured at several facilities [3] is related to $\vec{S}_g$ in Eq. (1) in the temporal gauge in the infinite-momentum frame of the nucleon [23]. From our discussion, ΔG is not the gauge-invariant gluon spin S_g'' that we construct here.

(v) Beth made a direct measurement of the photon spin over 70 years ago [10]. Detection and manipulation of the photon orbital angular momentum have also been carried out recently and have become a hot topic due to their potential application in quantum information processing [11–16]. These measurements can be straightforwardly interpreted with the operators in Eq. (6), via its equivalence to Eq. (4) in the Coulomb gauge. This should encourage the investigation of the picture of the nucleon spin in terms of the gauge-invariant, physically meaningful decomposition in Eq. (12), which is completely analogous to Eq. (6) for QED. Experimentally, the free-beam-based photon measurements can certainly not be extended to gluons directly, and appropriate (even ingenious) methods for measuring L_q'', S_g'', and L_g'' will have to be invented; but the clear physical meanings and explicit gauge invariance of these quantities guarantee at least that there can be pertinent theoretical calculations of them, especially in lattice QCD.

(vi) From the correct, gauge-invariant angular momentum expression in Eq. (6), we can read out the correct electromagnetic momentum *density* to be $E^i\vec{\nabla}A^i_{\rm phys}$, instead of the renowned Poynting vector $\vec{E}\times\vec{B}$. The latter actually includes a spin current and can be unambiguously distinguished from the purely mechanical momentum $E^i\vec{\nabla}A^i_{\rm phys}$ by delicate measurement [24]. In QCD, $\vec{E}^a\times\vec{B}^a$ leads to a picture that gluons carry half of the nucleon momentum on the light cone [25]. This picture may therefore need to be revised. Similarly to the situation for the angular momentum, the momentum operators we propose transform properly under spatial translation and rotation, and next, we will study how they transform under boost by computing their commutators with the boost generators via canonical quantization.

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