Perturbative quantum gauge invariance: where the ghosts come from

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Abstract: A condensed introduction to quantum gauge theories is given in the perturbative S-matrix framework, with path-integral methods used nowhere. This approach emphasizes the fact that it is not necessary to start from classical gauge theories that are then subject to quantization: it is possible, instead, to recover the classical group structure and coupling properties from purely quantum-mechanical principles. As a main tool, we use a free-field version of the Becchi–Rouet–Stora–Tyutin gauge transformation, which contains no interaction terms related to a coupling constant. This free gauge transformation can be formulated in an analogous way for quantum electrodynamics, Yang–Mills theories with massless or massive gauge bosons, and quantum gravity.

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Résumé : Nous présentons une introduction concise des théories quantiques de jauge dans le cadre perturbatif de la matrice S ; aucune intégrale de chemin n'apparaît. Cette approche insiste sur le fait qu'il n'est pas nécessaire de partir de théories classiques de jauge qui sont alors soumises à la quantification, mais qu'il est possible de retrouver la structure classique de groupe et les propriétés de couplage à partir de principes purement quantiques. Notre outil central est une version pour champ libre de la transformation de jauge de Becchi–Rouet–Stora–Tyutin, qui ne contient aucun terme d'interaction relié à la constante de couplage. Cette transformation de jauge libre peut être formulée de façon similaire pour l'électrodynamique quantique, les théories de Yang–Mills avec bosons (massifs ou non) et la gravité quantique.

[Traduit par la Rédaction]

1. Introduction

It is well known that gauge theories play a fundamental role in modern quantum field theory. From this observation one might conclude that gauge invariance is a physical mechanism inherent in many interactions. But this is not the case. Gauge invariance is, rather, a mathematical artifact that stems from the way we formulate (quantum) field theory. The presence of the artifact is, admittedly, very helpful in achieving a consistent formulation of many quantum field theories. As in general relativity, where we are free to choose the coordinate system according to our taste, we have some freedom in dealing with field theories. The free quantum fields that are used in perturbation theory to calculate physical quantities

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such as cross sections simply provide a "coordinatization" of the problem under consideration, and they are no less and no more "physical" than a coordinate system is.

One may illustrate this point with a simple observation. Massless particles with spin have only two degrees of freedom. Photons, for example, appear only in two helicity states. Such states are called "physical" in this paper, whereas timelike or longitudinal photons, which are an unavoidable by-product of covariant quantization, are called "unphysical". But, if we take into account that one can introduce running coupling constants and running masses into interacting field theories, it becomes clear that also "physical" particles such as quarks are merely mathematical constructions; we are always free to change the structure of the Fock space underlying our calculations by renormalizing the mass of the quark asymptotic states. It is, therefore, meaningless to ask how a composite particle can be decomposed into free "naked" particle states with a well-defined mass. What one really should do is calculate the vacuum expectation values of products of local interacting fields in a nonperturbative manner. From these distributions, it is, in principle, possible to reconstruct the true physical Hilbert space, as is claimed by the reconstruction theorem of Wightman [1]. (This is indeed a difficult task, which has been performed only for exotic cases, such as quantum field theories in $1 + 1$ space-time dimensions [2–5].)

It is not the intention of this introduction to describe completely all aspects of the arbitrariness in the formulation of quantum field theory. For mathematical details, we must refer to the literature. But since we are working in a strictly perturbative sense by using free-field operators only, the whole formalism used in this paper can be presented in a fully mathematical manner if necessary.

The structure of this paper is as follows: First, we start with the free classical electromagnetic field (or more precisely, with the classical gauge theory of a massless spin-1 field), for which the basic issues of classical gauge invariance are explained. Then the electromagnetic field is subjected to quantization, and we lift the gauge transformation on the quantum level. It is explained how the quantum gauge transformation, which is the free-field analogue of the full Becchi–Rouet–Stora–Tyutin (BRST) transformation [6, 7], can be applied to quantum chromodynamics (QCD) along the same lines as for quantum electrodynamics (QED). As a further step, the method is extended to massive gauge theories, where the Higgs field is involved. Finally, we outline how quantum gauge invariance can be formulated for quantum gravity.

2. The classical electromagnetic field

The equation of motion for the noninteracting vector potential A^μ in electrodynamics can be derived from the Lagrangian

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} = \frac{1}{2} \left(\boldsymbol{E}^2 - \boldsymbol{B}^2 \right) \tag{1}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the electromagnetic field strength tensor that can be expressed directly in terms of the components of the electric and magnetic fields $\boldsymbol{E}$ and $\boldsymbol{B}$. From the Euler–Lagrange equations

$$\partial_\nu \frac{\delta \mathcal{L}}{\delta \partial_\nu A_\mu} - \frac{\delta \mathcal{L}}{\delta A_\mu} = 0 \tag{2}$$

one then derives the wave equation

$$\partial_\nu \partial^\nu A_\mu - \partial_\mu \partial_\nu A^\nu = 0 \tag{3}$$

A problem arises from the fact that the physically measurable electromagnetic fields $\boldsymbol{E}$ and $\boldsymbol{B}$ remain unchanged if the vector potential is subject to a gauge transformation expressed by a real scalar field u $(x = (x^0, \boldsymbol{x}))$ given by

$$A_\mu(x) \to A_\mu(x) + \partial_\mu u(x) \tag{4}$$

In other words, there is a redundancy in the local description of the electromagnetic fields by a vector potential, aside from global topological information that may be contained in the potential, as in the case described by Aharonov and Bohm [8]. From the mathematical point of view, we generally assume that the objects we are dealing with "behave well," that is, that A_μ and u are differentiable and behave at large spatial distances in such a way as to make physical quantities such as the total energy of the field configuration finite.

The possibility of transforming the vector potential without changing its physical content allows us to impose *gauge conditions*. Because of its manifestly covariant form, a very popular choice is the Lorentz gauge condition, $\partial_\mu A^\mu = 0$. This condition can be enforced by transforming the initial vector potential according to (4) with a field u that satisfies

$$\Box u = \partial_\mu \partial^\mu u = -\partial_\mu A^\mu \tag{5}$$

Then the new transformed field satisfies the simple wave equation

$$\Box A^\mu = \partial_\nu \partial^\nu A^\mu = 0 \tag{6}$$

But the vector potential is not completely determined by the Lorentz gauge condition. It is still possible to apply a gauge transformation to the vector potential if u satisfies the wave equation $\partial_\nu \partial^\nu u = 0$, in such a way that the transformed vector potential is still in Lorentz gauge. In what follows, we will call the field u, which is somehow related to the unphysical degrees of freedom of the vector potential in Lorentz gauge, a "ghost field". The reason will become clear at a later stage.

It is important to note that the equation of motion for the vector potential can be manipulated by a modification of the Lagrangian according to an early observation of Fermi [9]. Adding a *gauge-fixing term* to the Lagrangian

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{2} \xi (\partial_\mu A^\mu)^2 \tag{7}$$

(here ξ is an arbitrary real parameter) leads to the equation of motion

$$\Box A_\mu - (1 - \xi) \partial_\mu \partial_\nu A^\nu = 0 \tag{8}$$

One may argue that the gauge fixing does not change the physical content of the Lagrangian, since we may enforce the Lorentz gauge condition $\partial_\mu A^\mu = 0$, and then the gauge-fixing term vanishes in the Lagrangian. For the special choice $\xi = 1$, we recover the wave equation (6). This choice is often referred to as the *Feynman gauge*, although this terminology is a bit misleading. We must clearly distinguish between (i) the gauge fixing (for instance, the Feynman gauge), which fixes the Lagrangian and determines the form of the wave equation, and (ii) the choice of a gauge condition for the vector potential (for instance, the Lorentz gauge), which reduces the redundancy originating from the use of a vector potential as a basic field. It is possible to impose more general (nonlinear) gauge-fixing conditions, for example, by adding a term $\sim (\partial_\mu A^\mu)^4$ to the Lagrangian, but we restrict ourselves to the most important cases here. We conclude this discussion of gauge fixing with the remark that it is indeed necessary to add appropriate gauge-fixing terms to the free Lagrangian (1), since otherwise problems arise in the construction of the free-photon propagator.

Up to now, the discussion of the electromagnetic field has been completely classical. In the next section, we will consider a quantized version of the free electromagnetic field. For the field operator $A_\mu(x)$, we will use the Feynman gauge, in such a way that the operator obeys the simplest equation of motion (6). All calculations could be performed in a strictly analogous way for arbitrary ξ gauges, but the choice $\xi = 1$ has obviously notational advantages [10]. Strictly speaking, each choice of ξ leads after quantization to a different quantum field theory with different Fock spaces and field operators. But physical observables, for instance cross sections, should be independent of the gauge fixing.

3. Quantization of free fields

It is well known that a free massless Hermitian scalar field $\varphi(x)$ can be represented by

$$\varphi(t, \boldsymbol{x}) = (2\pi)^{-3/2} \int \frac{\mathrm{d}^3 k}{\sqrt{2\omega}} \left(a(\boldsymbol{k})\, \mathrm{e}^{-i(\omega t - \boldsymbol{k}\boldsymbol{x})} + a(\boldsymbol{k})^\dagger\, \mathrm{e}^{i(\omega t - \boldsymbol{k}\boldsymbol{x})} \right) \tag{9}$$

where $\omega = |\boldsymbol{k}|$, and where the creation and annihilation operators satisfy the commutation relations

$$\left[a(\boldsymbol{k}),\ a(\boldsymbol{k}')^\dagger \right] = \delta^{(3)}(\boldsymbol{k} - \boldsymbol{k}') \tag{10}$$

$$\left[a(\boldsymbol{k}),\ a(\boldsymbol{k}') \right] = \left[a(\boldsymbol{k})^\dagger,\ a(\boldsymbol{k}')^\dagger \right] = 0 \tag{11}$$

We write † for the adjoint with respect to a positive-definite scalar product, allowing the operators to be represented in the usual way in a Fock space with unique vacuum. We write $\delta^{(3)}$ for the three-dimensional Dirac distribution.

We now try to quantize the vector potential $A^\mu(x)$ as four independent real scalar fields

$$A^\mu(t, \boldsymbol{x}) = (2\pi)^{-3/2} \int \frac{\mathrm{d}^3 k}{\sqrt{2\omega}} \left(a^\mu(\boldsymbol{k})\, \mathrm{e}^{-i(\omega t - \boldsymbol{k}\boldsymbol{x})} + a^\mu(\boldsymbol{k})^\dagger\, \mathrm{e}^{i(\omega t - \boldsymbol{k}\boldsymbol{x})} \right) \tag{12}$$

naively assuming the commutation relations for the creation and annihilation operators to be

$$\left[a^\mu(\boldsymbol{k}),\ a^\nu(\boldsymbol{k}')^\dagger \right] = \delta_{\mu\nu} \delta^{(3)}(\boldsymbol{k} - \boldsymbol{k}'), \qquad \left[a^\mu(\boldsymbol{k}),\ a^\nu(\boldsymbol{k}') \right] = \left[a^\mu(\boldsymbol{k})^\dagger,\ a^\nu(\boldsymbol{k}')^\dagger \right] = 0 \tag{13}$$

The condition $\Box A^\mu = 0$ is automatically satisfied according to (12), since the space-time dependence of the field operator is given by the plane-wave terms $\exp(\pm ikx) = \exp(\pm i(\omega t - \boldsymbol{k}\boldsymbol{x}))$. Here δ is the Kronecker delta of the indices μ, ν.

A calculation shows that the free massless Hermitian scalar field φ satisfies the commutation relation

$$[\varphi(x),\ \varphi(y)] = -iD(x - y) \tag{14}$$

where $D(x - y)$ is the (massless) Pauli–Jordan distribution

$$D(x) = \frac{i}{(2\pi)^3} \int \mathrm{d}^4 k\ \delta(k^2) \mathrm{sgn}(k^0)\, \mathrm{e}^{-ikx} = \frac{1}{2\pi} \mathrm{sgn}(x^0) \delta(x^2) \tag{15}$$

The Pauli–Jordan distribution satisfies the distributional identity

$$\partial_0 D(x)|_{x_0=0} = \delta^{(3)}(\boldsymbol{x}) \tag{16}$$

This implies the equal-time commutation relation, for a scalar field φ and its canonical momentum $\pi = \dot{\varphi}$,

$$[\varphi(x),\ \dot{\varphi}(y)]\,|_{x_0=y_0} = i\delta^{(3)}(\boldsymbol{x} - \boldsymbol{y}) \tag{17}$$

which is often taken as the starting point for the quantization of the scalar field. The distribution $D(x - y)$ was introduced by Pauli and Jordan in 1928, when they performed the first covariant quantization of the radiation field [11].

The naive choice (12) poses a problem since the commutation relations

$$\left[A^\mu(x),\ A^\nu(y) \right] = -i\delta_{\mu\nu} D(x - y) \tag{18}$$

are not covariant. A simple way to remedy this defect is to change the definition of A^0 to

$$A^0(x) = (2\pi)^{-3/2} \int \frac{d^3k}{\sqrt{2\omega}} \left(a^0(\boldsymbol{k})\, e^{-ikx} - a^0(\boldsymbol{k})^\dagger\, e^{ikx} \right) \tag{19}$$

that is, to make A^0 a skew-adjoint, rather than a self-adjoint, operator. Another strategy is to introduce a Fock space with negative norm states, as proposed by Gupta and Bleuler [12, 13]. The commutation relations then become

$$\left[A^\mu(x),\ A^\nu(y)\right] = i g^{\mu\nu} D(x-y) \tag{20}$$

We have introduced a non-Hermitian field to save the Lorentz symmetry of the theory, and therefore one might expect problems with the unitarity of the QED S-matrix. But no problems arise, a fact which is related to the gauge symmetry of the theory.

A concluding remark is in order here. It is possible to avoid unphysical polarization states by quantizing the photon field in radiation gauge, as expressed classically by the conditions

$$A^0 = 0, \qquad \nabla \cdot \boldsymbol{A} = 0 \tag{21}$$

The (quantized) photon-field operator contains then only physical (transverse) polarizations

$$A^0 = 0, \qquad \boldsymbol{A} = (2\pi)^{-3/2} \int \frac{d^3k}{\sqrt{2\omega}} \sum_{\lambda=1,2} \boldsymbol{\epsilon}\,(\boldsymbol{k},\lambda) \left[a(\boldsymbol{k},\lambda)\, e^{-ikx} + a^\dagger(\boldsymbol{k},\lambda)\, e^{ikx} \right] \tag{22}$$

with

$$\boldsymbol{\epsilon}\,(\boldsymbol{k},\lambda) \cdot \boldsymbol{\epsilon}\,(\boldsymbol{k},\lambda') = \delta_{\lambda\lambda'}, \qquad \boldsymbol{\epsilon}\,(\boldsymbol{k},\lambda) \cdot \boldsymbol{k} = 0 \tag{23}$$

and standard commutation relations for a and $a^\dagger$. But this is only seemingly an advantage, because manifest Lorentz symmetry is lost in (22), and no general strategy is known for dealing with the renormalization of divergent higher order contributions in interacting theories without the guiding help of Lorentz symmetry. We, thus, are obliged make the choice between using unphysical particles, but also having manifest Lorentz covariance in our calculations, or working only on a physical Fock space, but having no consistent scheme at hand for regularizing loop diagrams in perturbative calculations.

4. A simple version of a quantum gauge transformation

We now introduce a quantized version of the classical gauge transformation for the free vector potential

$$A^\mu \to A^\mu + \partial^\mu u, \qquad \Box u = 0 \tag{24}$$

Of course there exist different approaches for the treatment of gauge invariance in quantum field theory, but the approach presented here is quite simple and does the job.

As a first step, we define the gauge transformation operator or *gauge charge* Q

$$Q = \int\limits_{x_0=\text{const.}} d^3x\ \partial_\mu A^\mu(x) \overset{\leftrightarrow}{\partial_0} u(x) \tag{25}$$

It is sufficient for the moment to consider u as a real C-number field. In the case of QCD, u will necessarily become a Fermionic scalar field. It can be shown that Q is a well-defined operator on the

Fock space generated by the creation and annihilation operators according to (13). It is not important over which spacelike plane the integral in (25) is taken, since Q is time independent

$$\dot{Q} = \int\limits_{x_0=\text{const.}} \mathrm{d}^3x \left(-\partial_0^2\partial_\mu A^\mu u + \partial_\mu A^\mu \partial_0^2 u\right) = \int\limits_{x_0=\text{const.}} \mathrm{d}^3x \ \left(-\triangle\, \partial_\mu A^\mu u + \partial_\mu A^\mu \triangle\, u\right) = 0 \tag{26}$$

This formal proof uses the wave equation and partial integration. Another way to show the time independence of the gauge charge is to show that the *gauge current*, defined by

$$j_g^\mu = \partial_\nu A^\nu \overleftrightarrow{\partial^\mu} u, \qquad Q = \int \mathrm{d}^3x j_g^0 \tag{27}$$

is conserved

$$\partial_\mu j_g^\mu = \partial_\mu(\partial_\nu A^\nu \partial^\mu u - \partial^\mu \partial_\nu A^\nu u) = 0 \tag{28}$$

A crucial property of the gauge charge is expressed by the commutator with A^μ, which is a C-number

$$\left[Q,\ A^\mu(x)\right] = i\partial^\mu u(x) \tag{29}$$

All higher commutators, for instance

$$\left[Q,\ \left[Q,\ A^\mu(x)\right]\right] = 0 \tag{30}$$

vanish for obvious reasons. The reader is invited to check the commutation relation (29). (An outline of the calculation can be found in Appendix A.) We, therefore, have

$$\begin{aligned} \mathrm{e}^{-i\lambda Q} A^\mu\, \mathrm{e}^{+i\lambda Q} &= A^\mu - \frac{i\lambda}{1!}[Q,\ A^\mu] - \frac{\lambda^2}{2!}\left[Q,\ \left[Q,\ A^\mu\right]\right] + \cdots \\ &= A^\mu - i\lambda[Q,\ A^\mu] = A^\mu + \lambda\partial^\mu u \end{aligned} \tag{31}$$

that is, Q is a *generator* of gauge transformations.

5. Definition of perturbative quantum gauge invariance

We take the next step toward full QED and couple photons to electrons. In perturbative QED, the S-matrix is expanded as a power series in the coupling constant e. At first order, the interaction is described by the normally ordered product of free fields

$$\mathcal{H}_{\text{int}}(x) = -e : \bar{\Psi}(x)\gamma^\mu\Psi(x) : A_\mu(x) \tag{32}$$

where Ψ is the electron field operator. The S-matrix is then usually given in the literature by the formal expression (where T denotes time-ordering)

$$\begin{aligned} S &= \mathbf{1} + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int \mathrm{d}^4x_1 \ldots \mathrm{d}^4x_n\ T\left[\mathcal{H}_{\text{int}}(x_1)\ldots\mathcal{H}_{\text{int}}(x_n)\right] \\ &= \mathbf{1} + \sum_{n=1}^{\infty} \frac{1}{n!} \int \mathrm{d}^4x_1 \ldots \mathrm{d}^4x_n\ T_n(x_1, \ldots, x_n) \end{aligned} \tag{33}$$

Here we have introduced the time-ordered products T_n for notational simplicity, and we have

$$T_1(x) = -i\mathcal{H}_{\text{int}}(x) = ie : \bar{\Psi}(x)\gamma^\mu\Psi(x) : A_\mu(x) \tag{34}$$

Expression (33) is plagued by infrared and ultraviolet divergences (see Appendix E). We leave this technical problem aside and assume that the T_n are regularized, well-defined operator-valued distributions, symmetric in the space coordinates $x_1, \ldots, x_n$.

In the previous section, we used a real C-number field u to show how the gauge transformation can be lifted on the operator level. We assume now that u is a Fermionic scalar field, and additionally, we introduce an anti-ghost field $\tilde{u}$, which is *not* the Hermitian conjugate of u. The reason why we choose u, $\tilde{u}$ to be Fermionic, against all conventional wisdom that particles without spin are bosons, is very simple: Because bosonic ghosts do not allow one to formulate a consistent theory in the case of quantum chromodynamics, we start directly with the "correct" strategy. A second reason is that we want Q to be nilpotent ($Q^2 = 0$), allowing the definition of the physical Hilbert space as

$$\mathcal{F}_{\text{phys}} = \ker Q / \operatorname{ran} Q \tag{35}$$

(see Appendix C).

We give now a precise definition of perturbative quantum gauge invariance for QED. Our definition will work in a completely analogous way for QCD.

Let

$$Q := \int \mathrm{d}^3 x \, \partial_\mu A^\mu(x) \overset{\leftrightarrow}{\partial_0} u(x) \tag{36}$$

be the generator of (free-field) gauge transformations, called gauge charge for brevity. This Q was first introduced in a famous paper by Kugo and Ojima [14]. The positive and negative frequency parts of the free fields satisfy the {anti-}commutation relations

$$\left[A_\mu^{(\pm)}(x),\ A_\nu^{(\mp)}(y)\right] = i g_{\mu\nu} D^{(\mp)}(x-y) \tag{37}$$

$$\left\{u^{(\pm)}(x),\ \tilde{u}^{(\mp)}(y)\right\} = -i D^{(\mp)}(x-y) \tag{38}$$

and all other commutators vanish. Here $D^{\mp}$ are the positive and negative frequency parts of the massless Pauli–Jordan distribution with Fourier transforms

$$\hat{D}^{(\pm)}(p) = \pm \frac{i}{2\pi} \Theta\left(\pm p^0\right) \delta\left(p^2\right) \tag{39}$$

All the fields satisfy the Klein–Gordon equation with zero mass. Although, as already mentioned, we are working in Feynman gauge, the following discussion would go through with some technical changes in other covariant ξ gauges as well. Note that the quantum field A^μ does not satisfy $\partial_\mu A^\mu = 0$ on the whole Fock space, but only on the physical subspace. An explicit representation of the ghost fields is given by

$$u(x) = (2\pi)^{-3/2} \int \frac{\mathrm{d}^3 k}{\sqrt{2\omega}} \left(c_2(\boldsymbol{k})\, \mathrm{e}^{-ikx} + c_1^\dagger(\boldsymbol{k})\, \mathrm{e}^{ikx}\right) \tag{40}$$

$$\tilde{u}(x) = (2\pi)^{-3/2} \int \frac{\mathrm{d}^3 k}{\sqrt{2\omega}} \left(-c_1(\boldsymbol{k})\, \mathrm{e}^{-ikx} + c_2^\dagger(\boldsymbol{k})\, \mathrm{e}^{ikx}\right) \tag{41}$$

$$\left\{c_i(\boldsymbol{k}),\ c_j^\dagger(\boldsymbol{k}')\right\} = \delta_{ij} \delta^{(3)}(\boldsymbol{k} - \boldsymbol{k}'), \qquad i, j = 1, 2 \tag{42}$$

To see how the infinitesimal gauge transformation acts on the free fields, we have to calculate the commutators (see, ref. 15 and Appendix A)

$$\left[Q,\ A_\mu\right] = i \partial_\mu u; \qquad \{Q,\ u\} = 0; \qquad \{Q,\ \tilde{u}\} = -i \partial_\nu A^\nu; \qquad [Q,\ \Psi] = \left[Q,\ \bar{\Psi}\right] = 0 \tag{43}$$

The commutators of Q with the electron field are, of course, trivial, since the operators act on different Fock-space sectors. We need only the first and the last commutator in (43) here, with the others becoming important in the QCD case. From (31), we know that the commutator of Q with an operator gives the first-order variation of the operator, subject to a gauge transformation. Then we have for the first-order interaction T_1

$$[Q,\ T_1(x)] = -e : \bar{\Psi}(x)\gamma^\mu \Psi(x) : \partial_\mu u(x) \\ = i\partial_\mu(ie : \bar{\Psi}(x)\gamma^\mu \Psi(x) : u(x)) = i\partial_\mu T^\mu_{1/1}(x) \tag{44}$$

Here, we have used the fact that the electron current is conserved,

$$\partial_\mu : \bar{\Psi}\gamma^\mu \Psi := 0 \tag{45}$$

because Ψ satisfies the free Dirac equation. Note that the free electron field is *not* affected by the gauge transformation. We may call $T^\mu_{1/1} = ie : \bar{\Psi}\gamma^\mu \Psi : u$ the "Q-vertex" of QED. The generalization of (44) to nth order is

$$[Q, T_n\,(x_1, \ldots, x_n)] = i\sum_{l=1}^{n} \partial^{x_l}_\mu T^\mu_{n/l}\,(x_1, \ldots, x_n) = \text{(sum of divergences)} \tag{46}$$

where $T^\mu_{n/l}$ is again a mathematically well-defined version of the time-ordered product

$$T^\mu_{n/l}\,(x_1, \ldots, x_n) \text{ “}=\text{” } T\left(T_1(x_1)\ldots T^\mu_{1/1}(x_l)\ldots T_1(x_n)\right) \tag{47}$$

If one understands the second-order case, it is relatively easy to see how (46) comes about. This example is discussed in detail in Appendix D. We *define* (46) to be the condition of gauge invariance [15].

If we consider, for a fixed x_l, all terms in T_n with the external field operator $A_\mu(x_l)$

$$T_n\,(x_1, \ldots, x_n) =: t^\mu_l\,(x_1, \ldots, x_n)\, A_\mu(x_l) : + \cdots \tag{48}$$

(the dots represent terms without $A_\mu(x_l)$), then gauge invariance (46) requires

$$\partial^l_\mu \left[t^\mu_l\,(x_1, \ldots, x_n)\, u(x_l)\right] = t^\mu_l\,(x_1, \ldots, x_n)\partial_\mu u(x_l) \tag{49}$$

or

$$\partial^l_\mu t^\mu_l\,(x_1, \ldots, x_n) = 0 \tag{50}$$

that is, we obtain the Ward–Takahashi identities [16] for QED. Those identities express the implications of gauge invariance of QED, which is defined here on the operator level, by C-number identities for Green's distributions.

We have found the following important property of QED: There exists a symmetry transformation, generated by the gauge charge Q, that leaves the S-matrix elements invariant (since the gauge transformation only adds divergences in the analytic sense to the S-matrix expansion, and these divergences vanish, as explained in Appendix E, after integration over the coordinates $x_1, \ldots, x_n$).

The S-matrix "lives" on a Fock space $\mathcal{F}$ that contains physical and unphysical states. Unphysical single-photon states, for example, can be created by acting on the perturbative vacuum $|\Omega\rangle$ with timelike or longitudinal creation operators

$$a^0(\boldsymbol{k})^\dagger|\Omega\rangle, \qquad \sum_{j=1,2,3} k_j a^j(\boldsymbol{k})^\dagger|\Omega\rangle \tag{51}$$

and states that contain ghosts are always unphysical. The physical subspace $\mathcal{F}_{\text{phys}}$ is the space of states $|\Phi\rangle$ without timelike photons, longitudinal photons, or ghosts, that is,

$$a^0(\boldsymbol{k})|\Phi\rangle = 0, \qquad k_j a^j(\boldsymbol{k})|\Phi\rangle = 0, \qquad c_{1,2}(\boldsymbol{k})|\Phi\rangle = 0, \qquad \forall \boldsymbol{k} \tag{52}$$

Note that whereas the definition of the physical space is *not* Lorentz invariant, the definition (35) is.

The observation that QED is gauge invariant is interesting, but the true importance of gauge invariance lies in the fact that it allows one to prove, on a formal level, the *unitarity* of the S-matrix on the physical subspace (see the last paper of ref. 15). Because of the presence of the skew-adjoint operator A^0 or the presence of unphysical longitudinal and timelike photon states, the S-matrix is not unitary on the full Fock space, but it is on $\mathcal{F}_{\text{phys}}$. Although we do not give the algebraic proof here, we point out that gauge invariance is the basic prerequisite that ensures unitarity. A detailed discussion of this fact can be found in refs. 15, 17, and 18. We have introduced the ghosts only as a formal tool, since they "blow up" the Fock space unnecessarily and they do not interact with the electrons and photons. In QCD, however, the situation is not so trivial.

6. Quantum chromodynamics

As a further step, we now consider QCD without Fermions (quarks). The first-order coupling of the gluons that we obtain from the classical QCD Lagrangian is given (see Appendix B) by

$$\begin{aligned} T_1^A(x) &= i\frac{g}{2} f_{abc} : A_{\mu a}(x) A_{\nu b}(x) F_c^{\nu\mu}(x) : \\ &= ig f_{abc} : A_{\mu a}(x) A_{\nu b}(x) \partial^\nu A_c^\mu(x) :, \qquad a, b, c = 1, \ldots, 8 \end{aligned} \tag{53}$$

where $F_c^{\mu\nu} = \partial^\mu A_c^\nu - \partial^\nu A_c^\mu$ and f_{abc} are the totally antisymmetric structure constants of the gauge group SU(3). The asymptotic free fields satisfy the commutation relations

$$\left[A_{\mu a}^{(\pm)}(x),\ A_{\nu b}^{(\mp)}(y)\right] = i\delta_{ab} g_{\mu\nu} D^{(\mp)}(x-y) \tag{54}$$

and

$$\left\{u_a^{(\pm)}(x),\ \tilde{u}_b^{(\mp)}(y)\right\} = -i\delta_{ab} D^{(\mp)}(x-y) \tag{55}$$

and all other {anti-}commutators vanish. Defining the gauge charge as in (36) by

$$Q := \int \mathrm{d}^3x\ \partial_\mu A_a^\mu(x) \overset{\leftrightarrow}{\partial_0} u_a(x) \tag{56}$$

where summation over repeated indices is understood, we are led to the following commutators with the fields:

$$\left[Q,\ A_a^\mu\right] = i\partial^\mu u_a, \qquad \left[Q,\ F_a^{\mu\nu}\right] = 0, \qquad \{Q,\ u_a\} = 0, \qquad \{Q,\ \tilde{u}_a\} = -i\partial_\mu A_a^\mu \tag{57}$$

For the commutator of Q with T_1^A, we obtain

$$\begin{aligned} \left[Q,\ T_1^A(x)\right] &= ig f_{abc} : \left\{\left[Q,\ A_{\mu a}\right] A_{\nu b} \partial^\nu A_c^\mu + A_{\mu a}\left[Q,\ A_{\nu b}\right] \partial^\nu A_c^\mu + A_{\mu a} A_{\nu b}\left[Q,\ \partial^\nu A_c^\mu\right]\right\} : \\ &= -g f_{abc} : \left\{\partial_\mu u_a A_{\nu b} \partial^\nu A_c^\mu + \partial_\nu (A_{\mu a} u_b \partial^\nu A_c^\mu)\right\} : \end{aligned} \tag{58}$$

The last term is a divergence, but the first term spoils gauge invariance and, therefore, the unitarity of the theory. To restore gauge invariance, we must somehow compensate for the first term in (58).

We therefore consider the gluon–ghost coupling term

$$T_1^{\mu}(x) = igf_{abc} : A_{\mu a}(x) u_b(x) \partial^{\mu} \tilde{u}_c(x) : \tag{59}$$

For the commutator with Q, we get

$$\begin{aligned}\left[Q,\ T_1^{\mu}\right] &= ig : \left[Q,\ A_{\mu a}\right] u_b \partial^{\mu} \tilde{u}_c + A_{\mu a} \left\{Q,\ u_b\right\} \partial^{\mu} \tilde{u}_c - A_{\mu a} u_b \partial^{\mu} \left\{Q,\ \tilde{u}_c\right\} : \\ &= -gf_{abc} : \left\{\partial_{\mu} u_a u_b \partial^{\mu} \tilde{u}_c + A_{\mu a} u_b \partial^{\mu} \partial^{\nu} A_{\nu c}\right\} :\end{aligned} \tag{60}$$

Note that we can always decompose the commutator in a clever way that allows only anticommutators of Q to appear with the ghost fields and the commutators of Q to appear with the gauge fields. Taking the antisymmetry of f_{abc} and $: u_a u_b := - : u_b u_a :$ into account, we see that the first term is a divergence

$$f_{abc} : \partial_{\mu} u_a u_b \partial^{\mu} \tilde{u}_c := \frac{1}{2} f_{abc} \partial_{\mu} : u_a u_b \partial^{\mu} \tilde{u}_c : \tag{61}$$

because $\tilde{u}_c(x)$ satisfies the wave equation. The second term can be written as

$$-gf_{abc} : A_{\mu a} u_b \partial^{\mu} \partial^{\nu} A_{\nu c} := -gf_{abc} : \partial^{\nu} \left(A_{\mu a} u_b \partial^{\mu} A_{\nu c}\right) - \partial^{\nu} u_b A_{\mu a} \partial^{\mu} A_{\nu c} : \tag{62}$$

When the interchanges $a \leftrightarrow b$ and $\mu \leftrightarrow \nu$ are performed in the last term, it becomes equal to the first term in (58).

Hence, the combination

$$T_1(x) = igf_{abc} \left\{ \frac{1}{2} : A_{\mu a}(x) A_{\nu b}(x) F_c^{\nu\mu}(x) : - : A_{\mu a}(x) u_b(x) \partial^{\mu} \tilde{u}_c(x) : \right\} \tag{63}$$

leads to a gauge-invariant first-order coupling

$$[Q,\ T_1] = gf_{abc} : -\partial_{\nu} \left(A_{\mu a} u_b \left(\partial^{\nu} A_c^{\mu} - \partial^{\mu} A_c^{\nu}\right)\right) + \frac{1}{2} \partial_{\nu} \left(u_a u_b \partial^{\nu} \tilde{u}_c\right) : \tag{64}$$

In contrast with QED, the nonlinear self-interaction of the unphysical degrees of freedom of the gluons spoils gauge invariance. Coupling ghosts in an appropriate way to the gluons restores the consistency of the theory. That is why we need ghosts; they interfere destructively with the unphysical gluons and save the unitarity of the theory.

The first-order coupling given by (63) is in fact not the most general one, and it is also possible to construct a gauge-invariant first-order coupling with bosonic ghosts [15]. However, gauge invariance then breaks down at the second order of perturbation theory. Gauge invariance at order n is again defined by (46). We have discussed gauge invariance only at first order here. Proving that gauge invariance (and other symmetries of the theory) is not broken by renormalization is the "hard problem" of renormalization theory [19–21].

The four-gluon term $\sim g^2$, which also appears in the classical Lagrangian, is missing in T_1. This term appears as a necessary local normalization term at second order, and its structure is also fixed by perturbative gauge invariance. This underscores the fact that perturbative gauge invariance is strongly related to the formal expansion of the theory in powers of the coupling constant g.

We started this section by presupposing that the coupling of the gluons is already given by the classical Lagrangian. But perturbative gauge invariance is indeed a very restrictive condition: It fixes the interaction to a large extent. We outline here how this fact can be derived. Only a part of the derivation is given here, and it is not assumed that the reader will check the calculations in detail. A full discussion is given in ref. 18, and for further reading we recommend also ref. 22.

We start by describing the interaction of the massless gluons by the most general renormalizable Ansatz (the dimension of the interaction terms, in other words, being energy to the fourth power) with zero ghost number. (Coupling with non-zero ghost number would affect the theory only on the unphysical sector.) We note that

$$\begin{aligned}\tilde{T}_1(x) \quad = ig\Big\{ & \tilde{f}^1_{abc} : A_{\mu a}(x) A_{\nu b}(x) \partial^\nu A^\mu_c(x) : + \\ & \tilde{f}^2_{abc} : A_{\mu a} u_b \partial^\mu \tilde{u}_c : + \\ & \tilde{f}^3_{abc} : A_{\mu a} \partial^\mu u_b \tilde{u}_c : + \\ & \tilde{f}^4_{abc} : A_{\mu a} A^\mu_b \partial_\nu A^\nu_c : + \\ & \tilde{f}^5_{abc} : \partial_\nu A^\nu_a u_b \tilde{u}_c : \Big\}, \qquad \tilde{f}^4_{abc} = \tilde{f}^4_{bac}\end{aligned}$$

where the $\tilde{f}$ quantities are arbitrary real constants. This first-order coupling term is then antisymmetric with respect to the conjugation K defined in Appendix C.

Adding divergence terms to $\tilde{T}_1$ will not change the physics of the theory, since in (33) divergences get integrated out, and we assume that this property is not destroyed by the renormalization of the theory. Furthermore, the (anti-)commutator of Q with a divergence is also a divergence. Therefore, in the following, we can always calculate modulo divergences. We modify $\tilde{T}_1$ by adding $-(ig/4)(\tilde{f}^1_{abc} + \tilde{f}^1_{cba})\partial_\nu \; : \; A_{\mu a} A_{\nu b} A^\mu_c \; :$ and $-ig\tilde{f}^3_{abc}\partial_\mu \; : \; A^\mu_a u_b \tilde{u}_c \; :$ and arrive at a more compact, but equivalent, first-order coupling

$$\begin{aligned}T_1 \quad = ig\big\{ & f^1_{abc} : A_{\mu a} A_{\nu b} \partial^\nu A^\mu_c : + \\ & f^2_{abc} : A_{\mu a} u_b \partial^\mu \tilde{u}_c : + \\ & f^4_{abc} : A_{\mu a} A^\mu_b \partial_\nu A^\nu_c : + \\ & f^5_{abc} : \partial_\nu A^\nu_a u_b \tilde{u}_c : \big\}\end{aligned} \tag{65}$$

where

$$f^1_{abc} = -f^1_{cba}, \qquad f^4_{abc} = f^4_{bac} \tag{66}$$

The gauge variation of T_1 is

$$\begin{aligned}[Q,\, T_1] \quad = -g f^1_{abc} \quad & \Big\{ : \partial_\mu u_a A_{\nu b} \partial^\nu A^\mu_c + \\ & A_{\mu a} \partial_\nu u_b \partial^\nu A^\mu_c + \\ & A_{\mu a} A_{\nu b} \partial^\nu \partial^\mu u_c : \Big\} + \\ -g f^2_{abc} \quad & \Big\{ : \partial_\mu u_a u_b \partial^\mu \tilde{u}_c + \\ & A_{\mu a} u_b \partial^\mu \partial_\nu A^\nu_c : \Big\} + \\ -2g f^4_{abc} \quad & : \partial_\mu u_a A^\mu_b \partial_\nu A^\nu_c : + \\ -g f^5_{abc} \quad & : \partial_\nu A^\nu_a u_b \partial_\mu A^\mu_c :\end{aligned} \tag{67}$$

Gauge invariance requires that the gauge variation be a divergence. Hence, we make again a general

Ansatz

$$
\begin{aligned}
[Q,\ T_1] \quad = g\partial_\mu\big\{\, & g^1_{abc} : \partial^\mu u_a A_{\nu b} A^\nu_c : + \\
& g^2_{abc} : u_a A^\mu_b \partial_\nu A^\nu_c : + \\
& g^3_{abc} : \partial^\mu u_a u_b \tilde{u}_c : + \\
& g^4_{abc} : u_a u_b \partial^\mu \tilde{u}_c : + \\
& g^5_{abc} : \partial_\nu u_a A^\nu_b A^\mu_c : + \\
& g^6_{abc} : u_a \partial^\mu A^\nu_b A_{\nu c} : + \\
& g^7_{abc} : u_a \partial^\nu A^\mu_b A_{\nu c} :\big\}
\end{aligned} \tag{68}
$$

where $g^1_{abc} = g^1_{acb}$, $g^4_{abc} = -g^4_{bac}$. Comparing the terms in (67) and (68), we obtain a set of constraints for the coupling coefficients:

$$-f^1_{cab} = 2g^1_{abc} + g^6_{abc} \quad \text{from} \quad : \partial^\mu u \partial_\mu A_\nu A^\nu : \tag{69}$$

$$g^2_{abc} + g^5_{abc} = -2f^4_{abc} \quad : \partial^\mu u A_\mu \partial_\nu A^\nu : \tag{70}$$

$$g^2_{abc} + g^2_{acb} = -f^5_{bac} - f^5_{cab} \quad : u\partial_\nu A^\nu \partial_\mu A^\mu : \tag{71}$$

$$-f^2_{abc} = g^3_{abc} + 2g^4_{abc} \quad : \partial_\mu u u \partial^\mu \tilde{u} : \tag{72}$$

$$g^3_{abc} = g^3_{bac} \quad : \partial_\mu u \partial^\mu u \tilde{u} : \tag{73}$$

$$-f^1_{cba} - f^1_{bca} = g^5_{abc} + g^5_{acb} \quad : \partial_\mu \partial_\nu u A^\nu A^\mu : \tag{74}$$

$$-f^1_{acb} = g^5_{abc} + g^7_{abc} \quad : \partial_\mu u \partial_\nu A^\mu A^\nu : \tag{75}$$

$$g^6_{abc} = -g^6_{acb} \quad : u\partial_\mu A_\nu \partial^\mu A^\nu : \tag{76}$$

$$-f^2_{cab} = g^2_{acb} + g^7_{abc} \quad : u\partial_\mu \partial_\nu A^\mu A^\nu : \tag{77}$$

$$g^7_{abc} = -g^7_{acb} \quad : u\partial_\nu A^\mu \partial^\mu A^\nu : \tag{78}$$

From (74), (75), and (78), we readily derive

$$f^1_{abc} + f^1_{acb} - f^1_{bca} - f^1_{cba} = 0 \tag{79}$$

Combining this with (66), we obtain our first important result, that f^1_{abc} is *totally antisymmetric*. We note that g^1_{abc} is symmetric in b and c, and from (76) and (69), we conclude $g^1_{abc} = 0$ and $g^6_{abc} = -f^1_{abc}$.

We did not yet fully exploit gauge invariance. Additionally, upon taking into account that the gauge charge is nilpotent ($Q^2 = 0$) and that consequently

$$\{Q,\ [Q,\ T_1]\} = 0 \tag{80}$$

we obtain further relations that fix the interaction to

$$T_1 = T_1^{\mathrm{YM}} + T_1^{\mathrm{D}} \tag{81}$$

$$T_1^{\mathrm{YM}} = igf^1_{abc}\big\{: \frac{1}{2} A_{\mu a} A_{\nu b} F^{\nu\mu}_c : - : A_{\mu a} u_b \partial^\mu \tilde{u}_c :\big\} \tag{82}$$

$$T_1^{\mathrm{D}} = igf^5_{abc} : \partial_\nu A^\nu_a u_b \tilde{u}_c : \tag{83}$$

Here YM stands for "Yang–Mills" and D for "deformation", and $f^5_{abc} = -f^5_{cba}$.

We stop our analysis here for the sake of brevity. A detailed analysis of gauge invariance *at second order* shows [18] that the coupling coefficients f_{abc} must satisfy the Jacobi identity

$$f_{abc} f_{dec} + f_{adc} f_{ebc} + f_{aec} f_{bdc} = 0 \tag{84}$$

We are led, that is, to the nice result that the f_{abc} are structure constants of a Lie group. Note that whereas the Lie structure of gauge theories is usually presupposed, here it follows from basic symmetries of quantum field theory, namely, quantum gauge invariance (which is related to unitarity) and Lorentz covariance.

Finally, we are left with the term

$$T_1^{\mathrm{D}} = igf^5_{abc} : \partial_\nu A^\nu_a u_b \tilde{u}_c : \tag{85}$$

One can show that this interaction term, which contains only unphysical fields, does not contribute to the S-matrix on the physical sector.

The reason why maintaining gauge invariance at higher orders of the perturbation expansion is a nontrivial task can be understood qualitatively on a basic level. Commutators of free fields can be expressed by (derivatives of) Pauli–Jordan distributions, giving us, for example,

$$\left[\partial_\nu A^\nu(x), \partial_\mu A^\mu(y)\right] = ig^{\nu\mu}\partial^x_\nu \partial^y_\mu D(x-y) = -i\Box_x D(x-y) = 0 \tag{86}$$

But through the time-ordering process, Feynman-type propagators $\sim D_{\mathrm{F}}(x-y)$ satisfying the inhomogeneous wave equation

$$\Box D_{\mathrm{F}}(z) = -\delta^{(4)}(z) \tag{87}$$

appear in the amplitudes, instead of Pauli–Jordan distributions. In other words, because time-ordering does not commute with the analytic derivation, derivatives acting on Feynman propagators may generate “anomalous” local terms. The maintaining of gauge invariance may, therefore, require restrictions on the coupling structure also at higher orders. If it is not possible to modify the theory in such a way as to maintain gauge invariance, the theory is called *nonrenormalizable*. The result obtained by the analysis above can be considered an inversion of ’t Hooft’s famous result that Yang–Mills theories are renormalizable [23].

In this section, we focused on the purely gluonic part of QCD. A full discussion would include also the coupling of gluons to quarks, but all important features are contained in the present discussion.

7. Yang–Mills theories with massive gauge fields

In this section, we present a short discussion of a general Yang–Mills theory with massive gauge bosons. Free massive spin-1 fields with color index a satisfy the Proca equation

$$\Box A^\mu_a - \partial^\mu(\partial_\nu A^\nu_a) + m_a^2 A^\mu_a = 0 \tag{88}$$

Taking the divergence of (88), we find that the field automatically satisfies the Lorentz condition $\partial_\mu A^\mu_a = 0$. Again, we may quantize the fields as four independent scalar fields satisfying the wave equation

$$(\Box + m_a^2)A^\mu_a = 0 \tag{89}$$

The Lorentz condition is to be enforced on the Fock space as in the massless case, by selecting a physical subspace that contains the three allowed polarizations. Because of the mass of the gauge field, the definition of the gauge charge via (36) no longer leads to a nilpotent gauge charge. This can be restored by introducing scalar bosonic fields Φ_a with the same mass as the corresponding gauge field:

$$\left(\Box + m_a^2\right)\Phi_a = 0 \tag{90}$$

These fields, called Higgs ghosts or would-be Goldstone bosons, are unphysical. We demand that the free fields then satisfy the commutation relations

$$\left[A^\mu_a(x),\ A^\nu_b(y)\right] = i\delta_{ab}g^{\mu\nu}D_{m_a}(x-y) \tag{91}$$

$$\left[u_a(x),\ \tilde{u}_b(y)\right] = -i\delta_{ab} D_{m_a}(x-y) \tag{92}$$

$$[\Phi_a(x),\ \Phi_b(y)] = -i\delta_{ab} D_{m_a}(x-y) \tag{93}$$

where $D_{m_a}(x-y)$ are the usual Pauli–Jordan distributions

$$D_m(x) = \frac{i}{(2\pi)^3} \int d^4k\ \delta(k^2 - m^2)\mathrm{sgn}(k^0)\, \mathrm{e}^{-ikx} \tag{94}$$

for massive fields. We can proceed to define a nilpotent gauge charge by

$$Q := \int \mathrm{d}^3x\ (\partial_\mu A_a^\mu(x) + m_a \Phi_a(x))\ \overleftrightarrow{\partial_0}\ u(x) \tag{95}$$

Gauge variations are then obtained from the commutators

$$\left[Q,\ A_a^\mu\right] = i\partial^\mu u_a; \qquad \{Q,\ u_a\} = 0$$

$$\{Q,\ \tilde{u}_a\} = -i\left(\partial_\mu A_a^\mu + m_a \Phi_a\right); \qquad [Q,\ \Phi_a] = i m_a u_a \tag{96}$$

Because of the additional mass terms in the gauge variations (96), the coupling (63) that we obtained in the massless case, namely,

$$T_1(x) = igf_{abc}\left\{\frac{1}{2} : A_{\mu a}(x) A_{\nu b}(x) F_c^{\nu\mu}(x) : - : A_{\mu a}(x) u_b(x) \partial^\mu \tilde{u}_c(x) :\right\} \tag{97}$$

is now not gauge invariant. However, gauge invariance can be restored, at least at first order, if we add to T_1 a Higgs ghost coupling

$$T_1^\Phi = i\frac{g}{2} f_{abc}\left(\frac{m_b^2 + m_c^2 - m_a^2}{m_b m_c} : A_{\mu a}\Phi_b \partial^\mu \Phi_c : \right. \\ \left. + \frac{m_a^2 + m_c^2 - m_b^2}{m_a} : \Phi_a u_b \tilde{u}_c : + \frac{m_b^2 - m_a^2}{m_c} : A_{\mu a} A_b^\mu \Phi_c :\right) \tag{98}$$

for the case in which all masses are nonvanishing. But this is not the full story, because gauge invariance can be shown to break down again at second order under certain circumstances. As a consequence, a complete analysis of the situation is also necessary at higher orders. To illustrate the implications of gauge invariance, we present here the result of such an analysis for the case in which we have three different colors, assuming at least one of the three to be massive (because otherwise we would be dealing with a massless SU(2) Yang–Mills theory).

It is found that there exist two *minimal scenarios*, which are gauge invariant also at second order, whereas the coupling f_{abc} is equal to the completely antisymmetric tensor ε_{abc} for both cases.

One possibility is given by the case where two gauge boson are equally massive and the third one is massless. The correct coupling structure can be obtained from (98) by taking the limit $m_3 \to 0$ for $m_1 = m_2$. The corresponding massless Higgs ghost does not appear any more in the gauge charge Q, yielding a massless physical field.

The second possibility is given by the case in which all three gauge bosons are massive, and all masses are then equal. But it turns out, also, that it is necessary to introduce additional fields to save gauge invariance. Indeed, it is already sufficient to add one physical scalar to the theory (this, in other words, is the *minimal* solution): a Higgs boson. Gauge invariance fixes the structure of the coupling completely, but the mass of the Higgs remains a free parameter in the theory.

The two scenarios correspond to the classical picture of the two possible types of spontaneous symmetry breaking for an SU(2) Yang–Mills theory. In the first case, one couples a real SO(3) field triplet to the gauge fields. Two degrees of freedom of this triplet are "eaten up" by the gauge bosons, which become massive. In the second case, one couples a complex doublet (equivalent to four real fields) to the gauge bosons. Three degrees of freedom get absorbed by the gauge fields, which become massive, and one degree of freedom remains as a physical Higgs field. These two mechanisms are well described in many textbooks (see, for instance, ref. 24, Chapt. 8.3). A detailed discussion, adopting our present approach, of theories involving massive gauge fields such as the Z- and $W^{\pm}$-bosons can be found in refs. 25–29.

The interesting point of the free-field approach lies in the fact that it reverses the chain of arguments usually presented in the literature. Fields do not become massive because of the coupling to a Higgs field, but on the contrary, the existence of a Higgs field becomes necessary here because of the mass of the gauge bosons, and as a consequence of perturbative gauge invariance.

8. Quantum gravity (as a massless spin-2 gauge theory)

Throughout the discussion that follows, we should keep in mind that quantum gravity is a non-renormalizable theory, and not really understood to all orders in perturbation theory. But at least it is possible to discuss gauge invariance of the lowest orders [30, 31].

The general theory of relativity can be derived from the Einstein–Hilbert Lagrangian

$$\mathcal{L}_{\text{EH}} = -\frac{2}{\kappa^2}\sqrt{-g}R \tag{99}$$

where $R = g^{\mu\nu}R_{\mu\nu}$ is the Ricci scalar, g is the determinant of the metric tensor $g^{\mu\nu}$, and $\kappa^2 = 32\pi G$, G being Newton's gravitational constant. It is convenient to introduce Goldberg variables [32]

$$\tilde{g}^{\mu\nu} = \sqrt{-g}g^{\mu\nu} \tag{100}$$

Since we are working on a perturbative level, we expand the inverse metric $\tilde{g}^{\mu\nu}$ and assume that we have an asymptotically flat geometry

$$\tilde{g}^{\mu\nu} = \eta^{\mu\nu} + \kappa h^{\mu\nu} \tag{101}$$

Here $\eta^{\mu\nu} = \text{diag}(+1, -1, -1, -1)$ is the metric of Minkowski space-time. We used the more common symbol $g^{\mu\nu}$ for the flat-space metric in the previous sections, but use $\eta^{\mu\nu}$ in what follows so as to highlight the difference between η and g. We raise and lower all tensor indices with $\eta^{\mu\nu}$. The quantity $h^{\mu\nu}$ is a symmetric second-rank tensor field, describing gravitons after quantization. For notational convenience, we take it as a matter of indifference whether indices are up or down; the summation convention always makes clear what is meant. Formally, (99) can be expanded as an infinite power series

$$\mathcal{L}_{\text{EH}} = \sum_{j=0}^{\infty} \kappa^j \mathcal{L}_{\text{EH}}^{(j)} \tag{102}$$

in κ. The lowest order term $\mathcal{L}_{\text{EH}}^{(0)}$ is quadratic in $h^{\mu\nu}(x)$ and defines the wave equation of the free asymptotic fields. The linearized Euler–Lagrange equations of motion for $h^{\mu\nu}(x)$ are

$$\Box h^{\mu\nu}(x) - \frac{1}{2}\eta^{\mu\nu}\Box h(x) - h^{\mu\rho,\nu}_{,\rho}(x) - h^{\nu\rho,\mu}_{,\rho}(x) = 0 \tag{103}$$

where $h(x) = h^{\mu}_{\mu}(x)$, and where the commas denote partial derivatives with respect to the corresponding indices. This equation is invariant under classical gauge transformations of the form

$$h^{\mu\nu} \to h^{\mu\nu} + u^{\mu,\nu} + u^{\nu,\mu} - \eta^{\mu\nu}u^{\rho}_{,\rho} \tag{104}$$

where u^μ is a vector field satisfying the wave equation

$$\Box u^\mu(x) = 0 \tag{105}$$

As a consequence, quantum gauge invariance for gravity will be formulated with the help of (Fermionic) vector ghosts. This gauge transformation corresponds to the general covariance, in its linearized form, of the metric tensor $g_{\mu\nu}(x)$. The corresponding gauge condition, compatible with (104), is the Hilbert gauge, which obviously plays a role similar to the the Lorentz gauge condition for spin-1 fields:

$$h^{\mu\nu}_{,\mu} = 0 \tag{106}$$

The dynamical equation for the graviton field $h^{\mu\nu}$ then reduces to the wave equation

$$\Box h^{\mu\nu}(x) = 0 \tag{107}$$

The first-order term with respect to κ, $\mathcal{L}^{(1)}_{\mathrm{EH}}$, gives the trilinear self-coupling of the gravitons

$$\mathcal{L}^{(1)}_{\mathrm{EH}} = \frac{\kappa}{2}\, h^{\rho\sigma} \left(h^{\alpha\beta}_{,\rho} h^{\alpha\beta}_{,\sigma} - \frac{1}{2}\, h_{,\rho} h_{,\sigma} + 2\, h^{\alpha\rho}_{,\beta} h^{\beta\sigma}_{,\alpha} + h_{,\alpha} h^{\rho\sigma}_{,\alpha} - 2\, h^{\alpha\rho}_{,\beta} h^{\alpha\sigma}_{,\beta} \right) \tag{108}$$

There are many alternative derivations of this result (108), starting from massless tensor fields and requiring consistency with gauge invariance in some sense. A point of view similar to ours was taken by Ogievetsky and Polubarinov [33], who analyzed spin-2 theories by working with a generalized Hilbert-gauge condition to exclude the spin-1 part from the outset. They imposed an invariance under infinitesimal gauge transformations of the form

$$\delta h^{\mu\nu} = \partial^\mu u^\nu + \partial^\nu u^\mu + \eta^{\mu\nu} \partial_\alpha u^\alpha \tag{109}$$

and obtained Einstein's theory at the end. Wyss [34] instead considered the coupling to matter. Self-coupling of the tensor field (108) is then necessary for consistency. Wald [35] derived a divergence identity, equivalent to an infinitesimal gauge invariance of the theory. Einstein's theory is the only nontrivial solution of this identity. In quantum theory, the problem was studied by Boulware and Deser [36]. These authors require Ward identities associated with the graviton propagator for implementing gauge invariance. All authors obtain Einstein's theory as the unique classical limit if the theory is purely spin-2, without a spin-1 admixture.

In the discussion that follows, the free asymptotic field $h^{\mu\nu}$ is a symmetric tensor field of rank two, and u^μ and $\tilde{u}^\nu$ are ghost and anti-ghost fields on the background of Minkowski space-time. A symmetric tensor field has ten degrees of freedom, outnumbering the five independent components of a massive spin-2 field or the two degrees of freedom of the massless graviton field. The additional degrees of freedom can be eliminated on the classical level by imposing further conditions, but we will now quantize the graviton field and introduce the gauge-charge operator Q. The physical states in the full Fock space, which contains eight unphysical polarizations of the graviton and ghosts, can then be characterized directly with the help of the gauge charge, as in the case of a spin-1 field (see Appendix C and refs. 37–39).

The tensor field $h^{\mu\nu}(x)$ can be quantized as a massless field by

$$\left[h^{\alpha\beta}(x),\, h^{\mu\nu}(y) \right] = -i b^{\alpha\beta\mu\nu} D_0(x-y) \tag{110}$$

where $D_0(x-y)$ is again the massless Pauli–Jordan distribution and the tensor $b^{\alpha\beta\mu\nu}$ is constructed from the Minkowski metric $\eta^{\mu\nu}$ via

$$b^{\alpha\beta\mu\nu} = \frac{1}{2} \left(\eta^{\alpha\mu}\eta^{\beta\nu} + \eta^{\alpha\nu}\eta^{\beta\mu} - \eta^{\alpha\beta}\eta^{\mu\nu} \right) \tag{111}$$

An explicit representation of the field $h^{\mu\nu}(x)$ on the Fock space is given by

$$h^{\alpha\beta}(x) = (2\pi)^{-3/2} \int \frac{d^3k}{\sqrt{2\omega}} \left(a^{\alpha\beta}(\boldsymbol{k})\, e^{-ikx} + a^{\alpha\beta}(\boldsymbol{k})^{\dagger}\, e^{+ikx} \right) \tag{112}$$

Here we have $\omega = |\boldsymbol{k}|$ as usual, and $a^{\alpha\beta}(\boldsymbol{k}), a^{\alpha\beta}(\boldsymbol{k})^{\dagger}$ are annihilation and creation operators on a bosonic Fock space. One finds that these operators satisfy the commutation relations

$$\left[a^{\alpha\beta}(\boldsymbol{k}),\ a^{\mu\nu}(\boldsymbol{k}')^{\dagger} \right] = b^{\alpha\beta\mu\nu} \delta^{(3)}(\boldsymbol{k} - \boldsymbol{k}') \tag{113}$$

with all other commutators vanishing.

By analogy with the spin-1 theories, such as QCD, we may introduce a gauge-charge operator as

$$Q := \int\limits_{x^0=\text{const.}} d^3x\ h^{\alpha\beta}(x)_{,\beta} \overset{\leftrightarrow}{\partial}_0 u_\alpha(x) \tag{114}$$

For the construction of the physical subspace and to prove the unitarity of the S-matrix, we must have a nilpotent operator Q. Therefore, we have to quantize the ghost fields with anticommutators according to

$$\left\{ u^\mu(x),\ \tilde{u}^\nu(y) \right\} = i\eta^{\mu\nu} D_0(x - y) \tag{115}$$

All asymptotic fields obey the wave equation

$$\Box\, h^{\mu\nu}(x) = \Box\, u^\alpha(x) = \Box\, \tilde{u}^\beta(x) = 0 \tag{116}$$

We obtain the following commutators of the fundamental fields:

$$\left[Q,\ h^{\mu\nu} \right] = -\frac{i}{2} \left(u^\mu_{,\nu} + u^\nu_{,\mu} - \eta^{\mu\nu} u^\alpha_{,\alpha} \right) \tag{117}$$

$$[Q,\ h] = i u^\mu_{,\mu} \tag{118}$$

$$\left\{ Q,\ \tilde{u}^\mu \right\} = i h^{\mu\nu}_{,\nu} \tag{119}$$

$$\left\{ Q,\ u^\mu \right\} = 0 \tag{120}$$

From (117), we immediately get

$$\left[Q,\ h^{\mu\nu}_{,\mu} \right] = 0 \tag{121}$$

The result (117) agrees with the infinitesimal gauge transformations of the Goldberg variables, so that our quantization and choice of Q correspond to the classical framework.

Again, first-order gauge invariance means that $[Q,\ T_1]$ is a divergence in the sense of vector analysis, in other words that

$$[Q,\ T_1(x)] = i\partial_\mu T^\mu_{1/1}(x) \tag{122}$$

The definition of the nth-order gauge invariance then reads

$$[Q,\ T_n] = i \sum_{l=1}^{n} \frac{\partial}{\partial x^\mu_l} T^\mu_{n/l}(x_1, \ldots, x_l, \ldots, x_n) \tag{123}$$

As in the case of QCD, we are forced to add a ghost part to the self-coupling term of the gravitons. The first-order graviton coupling according to (108) is

$$\tilde{T}_1^h = \frac{i\kappa}{2} h^{\rho\sigma} \left(h^{\alpha\beta}_{,\rho} h^{\alpha\beta}_{,\sigma} - \frac{1}{2} h_{,\rho} h_{,\sigma} + 2 h^{\alpha\rho}_{,\beta} h^{\beta\sigma}_{,\alpha} + h_{,\alpha} h^{\rho\sigma}_{,\alpha} - 2 h^{\alpha\rho}_{,\beta} h^{\alpha\sigma}_{,\beta} \right) \tag{124}$$

By adding a physically irrelevant divergence to $\tilde{T}_1^h$, we obtain a more compact expression for the graviton interaction

$$T_1^h(x) = i\kappa : \left(\frac{1}{2} h^{\mu\nu} h^{\alpha\beta}_{,\mu} h^{\mu\nu} h^{\alpha\beta}_{,\nu} + h^{\mu\nu} h^{\nu\alpha}_{,\beta} h^{\mu\beta}_{,\alpha} - \frac{1}{4} h^{\mu\nu} h_{,\nu} h_{,\nu} \right) : \tag{125}$$

The ghost coupling turns out to be the one first suggested by Kugo and Ojima [40], namely,

$$T_1^u = i\kappa : \tilde{u}^{\nu}_{,\mu} \left(h^{\mu\nu}_{,\rho} u^{\rho} - h^{\nu\rho} u^{\mu}_{,\rho} - h^{\mu\rho} u^{\nu}_{,\rho} + h^{\mu\nu} u^{\rho}_{,\rho} \right) : \tag{126}$$

It is a nice detail that the four-graviton vertex that follows from the second-order term in (102) is also proliferated by gauge invariance at second order. It is, therefore, quite probable that also all higher vertex couplings appearing in (102) are proliferated by quantum gauge invariance. It is also possible to derive the couplings (124), (126) from perturbative gauge invariance, along the lines used in Sect. 6 for Yang–Mills theories. For this point and for further reading, we refer to a recent monograph, see, ref. 22.

Finally, we point out that it would be interesting to analyze the Higgs mechanism for massive gravity [41] in the framework presented above, and also to analyze it in connection with the dark-matter problem. A first step in this direction is presented in ref. 42.

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Appendix A. Commutator of the gauge charge Q with gauge fields

First we derive the distributional identity (16). The Pauli–Jordan distribution has an integral representation

$$D(x) = \frac{i}{(2\pi)^3} \int \mathrm{d}^4k \; \delta(k^2)\mathrm{sgn}(k_0)\, \mathrm{e}^{-ikx} \tag{A.1}$$

Using the identity

$$\delta(k^2) = \delta(k_0^2 - \boldsymbol{k}^2) = \frac{1}{2|k^0|}\Big(\delta(k^0 - |\boldsymbol{k}|) + \delta(k^0 + |\boldsymbol{k}|)\Big) \tag{A.2}$$

we obtain (exercising due care with $\mathrm{sgn}(k^0)$)

$$\partial_0 D(x) = \frac{i}{(2\pi)^3} \int \frac{\mathrm{d}^4 k}{2|k^0|} \Big(\delta(k^0 - |\boldsymbol{k}|) - \delta(k^0 + |\boldsymbol{k}|)\Big)\,(-ik^0)\,\mathrm{e}^{-ikx} \tag{A.3}$$

$$= \frac{1}{2(2\pi)^3} \int \mathrm{d}^3 k\, \Big(\mathrm{e}^{-i(|\boldsymbol{k}|x^0 - \boldsymbol{kx})} + \mathrm{e}^{-i(-|\boldsymbol{k}|x^0 - \boldsymbol{kx})}\Big) \tag{A.4}$$

Restricting this result to $x^0 = 0$, we get the desired result (16):

$$\partial_0 D(x)|_{x^0=0} = (2\pi)^{-3} \int \mathrm{d}^3 k\ \mathrm{e}^{+i\boldsymbol{kx}} = \delta^{(3)}(\boldsymbol{x}) \tag{A.5}$$

In a completely analogous way, one derives

$$\partial_0^2 D(x)|_{x^0=0} = 0, \qquad \boldsymbol{\nabla} D(x)|_{x^0=0} = 0 \tag{A.6}$$

Note that we always consider the well-defined differentiated distribution first, with the distribution then being restricted to a subset of its support.

As an example, we now investigate the commutator $[Q,\ A_\mu(y)]$, omitting the trivial color index. The commutator is given explicitly by

$$\big[Q,\ A_\mu(y)\big] = \Bigg[\int\limits_{x^0=y^0} \mathrm{d}^3 x\ \partial_\nu A^\nu(x)\ \overset{\leftrightarrow}{\partial_0^x}\ u(x),\ A_\mu(y)\Bigg] = i \int\limits_{x^0=y^0} \mathrm{d}^3 x\ \partial_\mu^x D(x-y)\ \overset{\leftrightarrow}{\partial_0^x}\ u(x) \tag{A.7}$$

We here make use of the freedom to choose any constant value for x^0, and so set $x^0 = y^0$, yielding $x^0 - y^0 = 0$ and letting us apply (16) and (A.6) in the sequel.

For $\mu = 0$ we have

$$\begin{aligned}[Q,\ A_0(y)] &= i \int\limits_{x^0=y^0} \mathrm{d}^3 x\ \partial_0^x D(x-y)\ \overset{\leftrightarrow}{\partial_0^x}\ u(x)\\ &= i \int\limits_{x^0=y^0} \mathrm{d}^3 x\ \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y})\,\partial_0^x u(x) = i\partial_0 u(y)\end{aligned} \tag{A.8}$$

where we have used the fact that the double timelike derivative of D vanishes on the integration domain according to (A.6). The result for the commutator of Q with the spacelike components of A is likewise obtained by using (16) and (A.6), and by shifting the gradient acting on the Pauli–Jordan distribution by partial integration on the ghost field.

Appendix B. The Becchi–Rouet–Stora–Tyutin transformation and its free-field version

The gluon vector potential can be represented by the traceless Hermitian 3×3 standard Gell-Mann matrices λ^a, $a = 1, ..., 8$:

$$A_\mu = \sum_{a=1}^{8} A_\mu^a \frac{\lambda^a}{2} =: A_\mu^a \frac{\lambda^a}{2} \tag{B.1}$$

The λ matrices satisfy the commutation and normalization relations

$$\left[\frac{\lambda^a}{2},\ \frac{\lambda^b}{2}\right] = i f_{abc}\frac{\lambda^c}{2}, \qquad \mathrm{tr}\,(\lambda^a\lambda^b) = 2\delta_{ab} \tag{B.2}$$

and the numerical values of the structure constants $f_{abc} = -f_{bac} = -f_{acb}$ can be found in numerous QCD textbooks. Since we are working with a fixed matrix representation, we do not care whether the color indices are upper or lower indices.

The natural generalization of the QED Lagrangian to the Lagrangian of purely gluonic QCD is

$$\mathcal{L}_{\text{gluon}} = -\frac{1}{2}\text{tr}\, G_{\mu\nu}G^{\mu\nu} = -\frac{1}{4}G^{a}_{\mu\nu}G^{\mu\nu}_{a} \tag{B.3}$$

with

$$G_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - ig\left[A_\mu,\ A_\nu\right] \tag{B.4}$$

or, using the first relation of (B.2),

$$G^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f_{abc} A^b_\mu A^c_\nu \tag{B.5}$$

It is an important detail that we are working with *interacting* classical fields here. The field-strength tensor, therefore, contains a term proportional to the coupling constant, in contrast to the free-field tensor $F^{\text{free}}_{\mu\nu} = \partial_\mu A^{\text{free}}_\nu - \partial_\nu A^{\text{free}}_\mu$ used in this paper. The Lagrangian $\mathcal{L}_{\text{gluon}}$ is invariant under classical local gauge transformations

$$A_\mu(x) \to U(x)A_\mu(x)U^{-1}(x) + \frac{i}{g}U(x)\partial_\mu U^{-1}(x) \tag{B.6}$$

where $U(x) \in SU(3)$.

We now extract the first-order gluon coupling from the Lagrangian. The Lagrangian

$$\mathcal{L}_{\text{gluon}} = -\frac{1}{4}\left[\partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f_{abc} A^b_\mu A^c_\nu\right]\left[\partial^\mu A^\nu_a - \partial^\nu A^\mu_a + g f_{ab'c'} A^\mu_{b'} A^\nu_{c'}\right] \tag{B.7}$$

obviously contains the “free-field” part (admittedly, the terminology is not really correct, since we are here dealing with interacting fields)

$$\mathcal{L}^{\text{free}}_{\text{gluon}} = -\frac{1}{4}\left[\partial_\mu A^a_\nu - \partial_\nu A^a_\mu\right]\left[\partial^\mu A^\nu_a - \partial^\nu A^\mu_a\right] \tag{B.8}$$

and the first-order interaction part is given by

$$\begin{aligned}\mathcal{L}^{\text{int}}_{\text{gluon}} &= -\frac{1}{4}\left[\partial_\mu A^a_\nu - \partial_\nu A^a_\mu\right]\left[g f_{ab'c'} A^\mu_{b'} A^\nu_{c'}\right] - \frac{1}{4}\left[g f_{abc} A^b_\mu A^c_\nu\right]\left[\partial^\mu A^\nu_a - \partial^\nu A^\mu_a\right] \\ &= -\frac{g}{2} f_{abc} A^b_\mu A^c_\nu \left[\partial^\mu A^\nu_a - \partial^\nu A^\mu_a\right] = -\frac{g}{2} f_{abc} A^a_\mu A^b_\nu \left[\partial^\mu A^\nu_c - \partial^\nu A^\mu_c\right] \\ &= g f_{abc} A^a_\mu A^b_\nu \partial^\nu A^\mu_c \end{aligned} \tag{B.9}$$

From this term follows the first-order interaction Ansatz $T^A_1 = i : \mathcal{L}^{\text{int}}_{\text{gluon}} :$ (53).

Since we are working in Feynman gauge, we add the corresponding gauge-fixing term $\mathcal{L}_{\text{gf}}$ to the Lagrangian. Additionally, we add a ghost term which leads to the ghost interaction (59). The total Lagrangian then becomes

$$\mathcal{L}_{QCD} = \mathcal{L}_{\text{gluon}} + \mathcal{L}_{\text{gf}} + \mathcal{L}_{\text{ghost}} = \mathcal{L}_{\text{gluon}} - \frac{1}{2}\left(\partial_\mu A^\mu_a\right)^2 + \partial^\mu \tilde{u}\left(\partial_\mu u_a - g f_{abc} u_b A_{\mu c}\right) \tag{B.10}$$

The classical ghosts are anticommuting Grassmann numbers; that is, $u^2 = \tilde{u}^2 = 0$, $u\tilde{u} = -\tilde{u}u$.

The BRST transformation is defined by

$$\delta A^a_\mu = i\lambda(\partial_\mu u_a - g f_{abc} u_b A_{\mu c}) \tag{B.11}$$

$$\delta \tilde{u}_a = -i\lambda \partial_\mu A^\mu_a \tag{B.12}$$

$$\delta u_a = \frac{g}{2}\lambda f_{abc} u_b u_c \tag{B.13}$$

where λ is a space-time-independent anticommuting Grassmann variable. The special property of the BRST transformation is the fact that the actions

$$S_{\text{gluon}} = \int \mathrm{d}^4x\, \mathcal{L}_{\text{gluon}}, \quad S_{\text{gf}} + S_{\text{ghost}} = \int \mathrm{d}^4x\, \left(\mathcal{L}_{\text{gf}} + \mathcal{L}_{\text{ghost}}\right), \quad S_{\text{total}} = S_{\text{gluon}} + S_{\text{gf}} + S_{\text{ghost}} \tag{B.14}$$

are all invariant under the transformation

$$\delta S_{\text{gluon}} = 0, \qquad \delta(S_{\text{gf}} + S_{\text{ghost}}) = 0 \tag{B.15}$$

The similarity of the free quantum gauge transformation introduced in this paper to the BRST transformation is obvious. One important difference is the absence of interaction terms $\sim g$. Furthermore, the free quantum gauge transformation is a transformation of free quantum fields, whereas the BRST transformation is a transformation of classical fields, which enter via path integrals when the theory is quantized. Finally, the free gauge transformation leaves the T_n quantities invariant up to divergences, whereas the BRST transformation is a symmetry of the full QCD Lagrangian. How the two symmetries are intertwined perturbatively is explained in ref. 20. A more rigorous axiomatic approach is discussed in refs. 19 and 43.

Appendix C. Some technical remarks concerning the gauge charge Q

Application of the Leibniz rule, for graded algebras, gives for the gauge charge in the case of massless spin-1 fields

$$Q^2 = \frac{1}{2}\{Q,\ Q\} = \frac{1}{2} \int\limits_{x_0=\text{const.}} \mathrm{d}^3x\ \partial_\nu A^\nu_a(x) \left\{ \overset{\leftrightarrow}{\partial}_{x_0} u_a(x),\ Q \right\} - \frac{1}{2} \int\limits_{x_0=\text{const.}} \mathrm{d}^3x \left[\partial_\nu A^\nu_a(x),\ Q\right] \overset{\leftrightarrow}{\partial}_{x_0} u_a(x) = 0 \tag{C.1}$$

making the operator nilpotent. This basic property of Q, which holds also in the massive case, and the so-called Krein structure on the Fock–Hilbert space [44, 45], allows one to prove unitarity of the S-matrix on the physical Hilbert space $\mathcal{F}_{\text{phys}}$, which is a subspace of the Fock–Hilbert space $\mathcal{F}$ containing also the unphysical ghosts and unphysical degrees of freedom of the vector field [46].

The physical Fock space can be expressed by the kernel and the range of Q [44, 46] as

$$F_{\text{phys}} = \ker Q / \operatorname{ran} Q = \ker \left\{Q,\ Q^\dagger\right\} \tag{C.2}$$

Again, this characterization of the physical space holds also for the massive spin-1 case and for the gauge charge (114) used for gravity. The Krein structure is defined by introducing a conjugation K

$$a_0(\boldsymbol{k})^K = -a_0(\boldsymbol{k})^\dagger, \qquad a_j(\boldsymbol{k})^K = a_j(\boldsymbol{k})^\dagger \tag{C.3}$$

so that $A^K_\mu = A_\mu$, and on the ghost sector

$$c_2(\boldsymbol{k})^K = c_1(\boldsymbol{k})^\dagger, \qquad c_1(\boldsymbol{k})^K = c_2(\boldsymbol{k})^\dagger \tag{C.4}$$

so that $u^K = u$ is K–self-adjoint and $\tilde{u}^K = -\tilde{u}$. Then Q is densely defined on the Fock–Hilbert space, becoming K-symmetric ($Q \subset Q^K$). Roughly speaking, the K-conjugation is the natural generalization of the usual Hermitian conjugation to the full (unphysical) Fock space.

A calculation shows that the anticommutator in (C.2) is essentially the number operator for unphysical particles, namely,

$$\left\{Q^{\dagger},\ Q\right\} = 2\int \mathrm{d}^3k\ \boldsymbol{k}^2 \left[b_1^{\dagger}(\boldsymbol{k})b_1(\boldsymbol{k}) + b_2^{\dagger}(\boldsymbol{k})b_2(\boldsymbol{k}) + c_1^{\dagger}(\boldsymbol{k})c_1(\boldsymbol{k}) + c_2^{\dagger}(\boldsymbol{k})c_2(\boldsymbol{k})\right] \tag{C.5}$$

with

$$b_{1,2} = \frac{\left(a_{\parallel} \pm a_0\right)}{\sqrt{2}}, \qquad a_{\parallel} = k_j a_j/|\boldsymbol{k}| \tag{C.6}$$

This implies (C.2).

The nilpotency of Q allows for standard homological notions [46]: Consider the field algebra $\mathcal{F}$ consisting of the polynomials in the (smeared) gauge and ghost fields and their Wick powers. Upon defining a gauge variation for a Wick monomial F according to

$$d_Q F \stackrel{\mathrm{def}}{=} QF - (-1)^{n_F} FQ \tag{C.7}$$

where n_F is the number of ghost fields in F, Q becomes a differential operator in the sense of homological algebra, and we have

$$d_Q^2 = 0 \quad \Longleftrightarrow \quad \{Q,\ [Q,\ F_{\mathrm{b}}]\} = [Q,\ \{Q,\ F_{\mathrm{f}}\}] = 0 \tag{C.8}$$

where F_{b} is a bosonic and F_{f} a fermionic operator and $d_Q(FG) = (d_Q F)G + (-1)^{n_F} F d_Q G$. For example, we get

$$d_Q :A_{\mu a} u_b \partial^{\mu}\tilde{u}_c: \,=\, :\left[Q,\ A_{\mu a}\right] u_b \partial^{\mu}\tilde{u}_c: + :A_{\mu a}\left[Q,\ u_b\right]\partial^{\mu}\tilde{u}_c: - :A_{\mu a} u_b \left\{Q,\ \partial^{\mu}\tilde{u}_c\right\}: \tag{C.9}$$

If $F = d_Q G$, then F is called a coboundary. The term (85)

$$\tilde{f}_{abc} :\partial_{\nu} A_a^{\nu} u_b \tilde{u}_c: \,=\, \frac{i}{2} d_Q \left(\tilde{f}_{abc} :\tilde{u}_a u_b \tilde{u}_c:\right) \tag{C.10}$$

is such a coboundary, which does not contribute to the physical QCD S-matrix.

Appendix D. Gauge invariance at *n*th order

A short discussion is given here to explain how the simple condition of gauge invariance at nth order in the coupling constant (46) emerges as a generalization from the first-order condition (44).

A thorough mathematical treatment of the subject would involve a discussion of operator-valued distributions, omitted here for brevity. Nevertheless, all mathematical steps presented in the treatment that follows can be put on a sound mathematical basis.

As a preliminary to our treatment, it is useful to recall some basic facts: Free quantum fields such as the free scalar field $\varphi(x)$ given by (9) are operator-valued distributions on a Fock–Hilbert space; that is, an operator $\varphi(g)$ is obtained after smearing out the field operator $\varphi(x)$ with a test function $g(x)$. This can be written *formally* as

$$\varphi(g) = \int \mathrm{d}^4x\ \varphi(x) g(x) \tag{D.1}$$

where $g \in \mathcal{S}(\mathbf{R}^4)$ is in the Schwartz space of infinitely differentiable and rapidly decreasing test functions. Furthermore, the tensor product $\varphi(x)\psi(y)$ of free fields is also an operator-valued distribution (as are normally ordered products of free fields), whereas the local product $\varphi(x)\varphi(x)$ is only defined after normal ordering. Although it makes no sense in general to speak of the "value" of a distribution at a single point, it can be convenient to treat distributions like ordinary functions because in many cases the less complex insight gained from such a simplification allows one to construct a full mathematical proof at a later stage. For this reason, we make such a simplification in the treatment that follows.

As mentioned in the body of this paper, the $T_n(x_1, \ldots, x_n)$ are well-defined time-ordered products of the first-order coupling $T_1(x)$, and they are expressed in terms of Wick monomials of free fields. The construction of the T_n requires some care: If the arguments $x_1, \ldots, x_n$ are all time-ordered, that is, if we have

$$x_1^0 > x_2^0 > \cdots > x_n^0 \tag{D.2}$$

then T_n is given simply by

$$T_n(x_1, \ldots, x_n) = T_1(x_1)T_1(x_2)\ldots T_1(x_n) \tag{D.3}$$

According to the definition (33), the $T_n(x_1, \ldots, x_n)$ can be considered symmetric in $x_1, \ldots, x_n$. Using this fact allows us, in principle, to obtain the operator-valued distribution T_n inductively everywhere except for the "complete diagonal" $\Delta_n = \{x_1 = \cdots = x_n\}$ [47]. The construction is inductive because subdiagrams with lower order appear in the construction of T_n. If T_n were a C-number distribution, we could make it a well-defined distribution for all $x_1, \ldots, x_n$ by extending the distribution from $\mathcal{R}^{4n}/\Delta_n$ to $\mathcal{R}^{4n}$. In the case of free-field operators, the problem can be reduced to a C-number problem by using the Wick expansion of the operator-valued distributions. The extension $T(x_1, \ldots, x_n)$ is, of course, not unique: it is ambiguous up to distributions with local support Δ_n. This ambiguity can be further reduced with the help of symmetries (in particular, gauge invariance) and power-counting theory, and it is this local ambiguity that shows up as ultraviolet divergences in Feynman-diagram calculations.

The concrete inductive construction of the T_n is discussed in detail in a famous paper of Epstein and Glaser [48] for scalar field theories, and is explained in a more pedagogical way in [49]. For many practical calculations, it is advantageous to work in momentum space, since the distributions, namely, the Green's functions that occur in the calculations, behave much more smoothly in p-space than in x-space. The work of Epstein and Glaser is based on a treatment in real space, whereas in ref. 49 practical calculations are performed in momentum space. An advantage of the real-space formulation is that it allows one to formulate a consistent renormalization theory on a curved physical background [50]. Interesting topics such as scale invariance, renormalization, and the renormalization group can also be treated in real space [51–53].

As a specific example, we consider the second-order contribution to the S-matrix given by

$$S_2 = \frac{1}{2!}\int \mathrm{d}^4x\,\mathrm{d}^4y\; T\left[T_1(x)T_1(y)\right] = \frac{1}{2}\int \mathrm{d}^4x\,\mathrm{d}^4y\; T_2(x,y) \tag{D.4}$$

We consider first the simple product $T_1(x)T_1(y)$ without time ordering. In this case we find

$$\begin{aligned}[Q,\ T_1(x)T_1(y)] &= [Q,\ T_1(x)]\,T_1(y) + T_1(x)\,[Q,\ T_1(y)] \\ &= i\partial_\mu T^\mu_{1/1}(x)T_1(y) + iT_1(x)\partial_\mu T^\mu_{1/1}(y)\end{aligned} \tag{D.5}$$

In considering the time-ordered product $T[T_1(x)T_1(y)]$, we have to distinguish three cases. In the first case, we have $x^0 > y^0$, and therefore $T[T_1(x)T_1(y)] = T_1(x)T_1(y)$. The second, somewhat less trivial, case is given by $x^0 < y^0$. We now find $T\,[T_1(x)T_1(y)] = T_1(y)T_1(x)$, and

$$\begin{aligned}[Q,\ T\,(T_1(x)T_1(y))] &= [Q,\ T_1(y)]\,T_1(x) + T_1(y)\,[Q,\ T_1(x)] \\ &= i\partial_\mu T^\mu_{1/1}(y)T_1(x) + iT_1(y)\partial_\mu T^\mu_{1/1}(x) \\ &= iT\left[\partial_\mu T^\mu_{1/1}(x)T_1(y)\right] + iT\left[T_1(x)\partial_\mu T^\mu_{1/1}(y)\right]\end{aligned} \tag{D.6}$$

Finally, we may have $x^0 = y^0$. If $(\boldsymbol{x} - \boldsymbol{y}) \neq \mathbf{0}$, in other words if x and y have a spacelike separation, then we may perform "a little" Lorentz transformation such that $x^0 > y^0$, and the discussion above applies. In the special case that $x = y$, gauge invariance is not trivially obtained. This is not astonishing, since this is the case on the diagonal $\Delta_2 = \{x = y\}$, where perturbation theory may fail to calculate time-ordered products of the first-order interaction. Requiring that gauge invariance hold also for $x = y$ leads to Ward–Takahashi identities in QED, and to the so-called Slavnov–Taylor identities for QCD.

The simplest example of such an identity is obtained from the vacuum polarization contribution to the QED S-matrix at second order, which can be written in the form

$$T_2^{vp}(x, y) =: A_\mu(x) t^{\mu\nu}(x - y) A_\nu(y) : \tag{D.7}$$

where $t^{\mu\nu}(x - y) = t^{\nu\mu}(x - y)$ is a C-number distribution. Operator gauge invariance requires

$$\begin{aligned}\left[Q,\ T_2^{vp}(x, y)\right] &= i\partial_\mu u(x) t^{\mu\nu}(x - y) A_\nu(y) + i A_\mu(x) t^{\mu\nu}(x - y)\partial_\nu u(y) \\ &= i\partial_\mu^x \left[u(x) t^{\mu\nu}(x - y) A_\nu(y)\right] + i\partial_\nu^y \left[A_\mu(x) t^{\mu\nu}(x - y) u(y)\right]\end{aligned} \tag{D.8}$$

and therefore

$$\partial_\mu^x t^{\mu\nu}(x - y) = \partial_\nu^y t^{\mu\nu}(x - y) = 0 \tag{D.9}$$

In momentum space, we get the C-number identity

$$k_\mu \hat{t}^{\mu\nu}(k) = k_\nu \hat{t}^{\mu\nu}(k) = 0 \tag{D.10}$$

and hence the vacuum polarization tensor is transversal.

Appendix E. The adiabatic limit

The perturbative expression (33) is problematic in that the time-ordered products T_n are operator-valued distributions after regularization, requiring smearing out by test functions. To be more precise in a mathematical sense, we introduce a test function $g_0(x) \in \mathcal{S}(\mathbf{R}^4)$, with $g_0(0) = 1$, and replace (33) with

$$S = \mathbf{1} + \sum_{n=1}^{\infty} \frac{1}{n!} \int \mathrm{d}^4x_1 \ldots \mathrm{d}^4x_n\ T_n\left(x_1, \ldots, x_n\right) g_0\left(x_1\right) \ldots g_0\left(x_n\right) \tag{E.1}$$

Here g_0 acts as an infrared regulator, which switches off the long-range part of the interaction in theories where massless fields are involved. In QED, for example, the emission of soft photons is switched by g_0, and as long as we do not take a so-called adiabatic limit $g_0 \to 1$, the elements of the S-matrix remain finite. One possibility for taking the adiabatic limit is scaling the switching function $g_0(x)$, that is, replacing $g_0(x)$ with $g(x) = g_0(\epsilon x)$ and taking the limit $\epsilon \to 0$, in such a way that g everywhere approaches the value 1. If the S-matrix is modified by a gauge transformation, operators which are divergences are added to the nth-order term T_n. Such a contribution can be written as

$$\begin{aligned}&\int \mathrm{d}^4x_1 \ldots \mathrm{d}^4x_n\ \partial_\mu^{x_l} O^{\cdots\mu\cdots}\left(x_1, \ldots, x_l, \ldots, x_n\right) g\left(x_1\right) \ldots g\left(x_l\right) \ldots g\left(x_n\right) \\ &\qquad = -\int \mathrm{d}^4x_1 \ldots \mathrm{d}^4x_n\ O^{\cdots\mu\cdots}\left(x_1, \ldots, x_l, \ldots, x_n\right) g\left(x_1\right) \ldots \partial_\mu^{x_l} g\left(x_l\right) \ldots g\left(x_n\right)\end{aligned} \tag{E.2}$$

In the adiabatic limit, the gradient $\partial_\mu^{x_l} g(x_l)$ vanishes. Unfortunately, this property of the scaling limit does not guarantee that the whole term (E.2) vanishes (see also refs. 54 and 55).

The infrared problem is not really understood in QCD; all proofs of unitarity in the literature have to be taken with a grain of salt because they are somehow avoiding the discussion of infrared problems.

A thorough perturbative approach to the construction of the *local* algebras of observables that avoids the adiabatic limit is given for QED in ref. 43 and (under the assumption that there are no anomalies) for non-Abelian gauge theories in ref. 19.