Eur. Phys. J. C 21, 175–179 (2001)
Digital Object Identifier (DOI) 10.1007/s100520100709

THE EUROPEAN
PHYSICAL JOURNAL C

On the gauge independence of the S-matrix

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Received: 27 April 2001 /
Published online: 6 July 2001 –

Abstract. The S-matrix is invariant with respect to the variation of any (global) parameter involved in the gauge-fixing conditions, if that variation is accompanied by a certain redefinition of the basis of polarization vectors. Renormalizability of the underlying gauge theory is not required. The proof is nonperturbative and, using the "extended" BRS transformation, quite simple.

1 Introduction

After half a century of quantum gauge theory still some confusion seems to prevail regarding the difference between gauge invariance and gauge independence. A closely related difficulty concerns the concept of a "physical observable". For example, to this day gauge invariance of a certain operator to some people implies that it is an "observable", despite the work of many authors many years ago [1] – mainly in the context of deep inelastic scattering of leptons – that renormalization introduces an unavoidable mixture with other (ghost-dependent) operators[1] in the gauge-fixed theory. The physical observables in that case, in a quite roundabout manner, become only one aspect of the gauge-invariant operators: only the anomalous dimensions of those operators enter as ingredients in the S-matrix element. Thus the gauge independence of the latter is the central issue, a topic usually just taken for granted in the literature. I am not aware of any experimental situation in which – from the point of view of quantum *field* theory, for which ordinary quantum mechanics, generalizing classical point particles, represents only a subdomain! – anything else than an S-matrix element provides the link between theory and experiment[2]. The literature on the gauge independence of that quantity is very scarce. Since the proof proposed by Costa and Tonin [3], apart from adapting their argument to a proof in the axial gauge [4] and to superfields [5] I am only aware of [6] where a proof for scattering of fermions in the standard model was given which uses the Nielsen identities [7]. However, at the time when e.g. first computations in quantum gravity, involving full back reaction of the background (at least in the spherically reduced case [8]) have become available, and when the issue of an S-matrix element in gravity [9] becomes important when scattering of particles through an intermediate "virtual black hole" can be considered in a specific gauge [10], the publication of a simple and nevertheless complete proof, which is not restricted to gauge theories based upon Lie groups, seems to be useful[3]. It uses the concept of extended BRS symmetry and the related Slavnov–Taylor identity for the generating function of Green functions [12] (Sect. 2), completely avoiding the detour [7] through Nielsen identities [8] which are identities determining the gauge dependence of one-particle-irreducible (1pi) vertices. Generically such identities are more important for questions related to renormalization and to the gauge dependence of anomalies [13], although they have shown their usefulness for the definition of mass, width of unstable particles, effective actions etc. [14].

The "physical" poles of the propagator yield the definition of the polarizations to be used in the S-matrix (Sect. 3). We assume the existence of such poles for massive particles. Gauge fields can be included after regularization by spontaneous symmetry breaking, if that mechanism is not provided by nature anyhow (as for the W- and Z-bosons).

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[1] A similar mechanism involving the gauge parameter-dependent operators works in the (ghost-free) axial and temporal gauges [2].

[2] In my view the definition of "observables" should also include a prescription of how to measure those quantities, e.g. the eigenvalues of hermitian operators in ordinary quantum mechanics. Take the total angular momentum of such a system: In order to measure it, one must let the system interact with some "external field" (here magnetic field) which is (weakly) coupled to that quantity. But then in the larger system, including that interaction, one again effectively has to calculate some S-matrix element, involving asymptotic initial and final states. In this sense the experimental preparation of the incoming system and the interactions with the detecting device are "asymptotic".

[3] I have been reminded a few times and especially recently [11] that such a simple proof, which has formed for many years part of my lectures on quantum field theory at the Vienna University of Technology, should be made available.

Our proof is outlined in Sect. 4, whereas possible limitations and extensions are discussed in the conclusions (Sect. 5).

2 Extended identity for Green functions

The argument will be based on the generating functional Z for Green functions which can be written as

$$Z^{(0)}(j,k) = \int (\mathrm{d}\phi_A) \exp \mathrm{i} L^{(0)}, \tag{1}$$

with the action (summation of indices includes integration)

$$L^{(0)} = L_{\mathrm{inv}} + L^{(0)}_{\mathrm{gf}} + j_A \phi_A + k_A (s\phi_A). \tag{2}$$

The symbol $\phi_A = (\phi_i, A_\alpha)$ comprises gauge fields, matter fields (ϕ_i) and auxiliary fields (A_α), appearing as a consequence of the gauge-fixing procedure. Because of the possible presence of fermions and of Faddeev–Popov (FP) ghosts grading should be taken into account:

$$\phi_A \phi_B = (-1)^{\mathrm{AB}} \phi_B \phi_A \tag{3}$$

In the exponent of (-1) for a (anti-)commuting field ϕ_A we set $(A = 1)$ $A = 0$. The bosonic nature of $L^{(0)}$ entails the same relation for the sources j_A. Gauge fixing leaves (2) invariant under the BRS transformation [15]

$$\delta\phi_A = \delta\lambda s\phi_A, \tag{4}$$

where $s^2 = 0$ on all ϕ_A and $\delta\lambda$ is a (global) anticommuting parameter. The explicit form of $s\phi_A$ need not be specified. According to Zinn-Justin [16] sources k_A for $s\phi_A$ have been introduced. Clearly $s\phi_A$ and thus k_A have grading $A+1$. For the gauge-fixing action $L^{(0)}_{\mathrm{gf}}$ we only need that it is BRS exact

$$L^{(0)}_{\mathrm{gf}} = s\Psi(\phi, p), \tag{5}$$

where the (anticommuting) functional Ψ depends by the gauge-fixing condition on gauge parameters which we take to be commuting (global) variables. It is sufficient to select one of them, called p, in what follows.

To give a concrete example, for the special case of linear inhomogeneous gauge fixing we may choose

$$\Psi = \bar{b}_\alpha F_{\alpha i} \phi_i - \frac{\beta}{2} \bar{b}_\alpha B_\alpha, \tag{6}$$

where $\bar{b}_\alpha$ is the antighost, related to the Nakanishi–Lautrup field B_α by $B_\alpha = s\bar{b}_\alpha, sB_\alpha = 0$, with $s\phi_i = D_{i\alpha}(\phi) c_\alpha$ containing the ghost field c_α and $D_{i\alpha}$ from the gauge transformation $\delta\phi_i = D_{i\alpha}\delta\omega_\alpha$. Equations (5) with (6) produce in this case the usual gauge- fixing term and the FP action. The gauge parameter p could be β or also some parameter in F_{α_i}. Actually the explicit form of Ψ in (6) will not be relevant below.

The idea of "extended" BRS transformation consists in including the gauge parameter p in the BRS operations, $sp = z, sz = 0$ or, equivalently, to introduce a new (nilpotent, $\sigma^2 = 0$) operation

$$\sigma = z \frac{\partial}{\partial p}, \tag{7}$$

because the (anticommuting) z obeys $z^2 = 0$ trivially.

The extended generating functional, depending on z is now

$$Z(j,k,z) = \int (\mathrm{d}\phi_A) \exp \mathrm{i} L, \tag{8}$$

where L differs from $L^{(0)}$ only by the replacement[4]

$$L^{(0)}_{\mathrm{gf}} = s\Psi \to L_{\mathrm{gf}} = (s+\sigma)\Psi. \tag{9}$$

The derivation of the Slavnov–Taylor identity proceeds as usual by the BRS transformation (4) inside the path integral (8). The only terms in L affected are the source term involving j_A and the new term with σ from (9):

$$0 = \int (\mathrm{d}\phi) [j_A \delta\lambda s\phi_A + \sigma\delta\lambda s\Psi] \exp \mathrm{i} L. \tag{10}$$

In (10) we have tacitly assumed BRS invariance of the measure $(\mathrm{d}\phi)$. This holds for gauge theories based upon Lie groups. But also in other cases a covariant measure can be constructed, introducing e.g. the famous factor $(-g)^{1/4}$ for diffeomorphism invariance for the path integral of matter fields in gravity [18]. The global parameter $\delta\lambda$ is (anti-)commuted to the left and dropped, $s\phi_A$ replaced by $\mathrm{i}^{-1}\delta/\delta k_A$ and $s\Psi$ by $L^{(0)}_{\mathrm{gf}}$ (cf. (5)).

Clearly a path integral like (1) or (8) is only meaningful if some kind of regularization is implied which, however, we do not have to specify. We shall not assume that the renormalization (with counterterms added to L) has been performed as yet. Therefore, the entire dependence on p still resides in $L^{(0)}_{\mathrm{gf}}$ (and nowhere else in $L^{(0)}$). Thus in the second term of (10) $s\Psi$ may be replaced even by the full extended L because $\sigma^2 = 0$. This term simply corresponds to the action of (7) on Z:

$$z \frac{\partial Z}{\partial p} = (-1)^A j_A \frac{\delta Z}{\delta k_A}. \tag{11}$$

Expanding $Z = Z^{(0)} + zZ^{(1)}$ the part linear in z of (11),

$$\frac{\partial Z^{(0)}}{\partial p} = (-1)^{A+1} j_A \frac{\delta Z^{(1)}}{\delta k_A}, \tag{12}$$

yields all the information needed below. At $j_A = 0$ from (12) immediately follows the gauge independence of the vacuum loop contribution $Z^{(0)}(j = k = 0) \equiv Z^{(0)}(0)$.

[4] This trick has been used successfully to also incorporate "external" (global) symmetries of the action in order to obtain e.g. consistency conditions for anomalies in a very compact manner [17].

For the Green functions with N external legs

$$G_{A_1\dots A_N} = \frac{(-\mathrm{i})^N}{Z^{(0)}(0)} \frac{\delta^N Z^{(0)}}{\delta j_{A_1}\dots\delta j_{A_N}}\bigg|_{j=k=0}. \quad (13)$$

Multiplication of (12) with the gauge-independent factor $[Z^{(0)}(0)]^{-1}$ and N-fold differentiation as in (13) at $j = k = 0$ leads to the identity

$$\frac{\partial G_{A_1\dots A_N}}{\partial p} = \sum_{\ell=1}^{N} (-1)^{1+\sum_{\nu=\ell}^{\nu=N} A_\nu} G^{(1)}_{A_1\dots \underline{A}_\ell \dots A_N}, \quad (14)$$

where $G^{(1)}$ is defined exactly like G, but with one of the j-legs replaced by a k-leg:

$$G^{(1)}_{A_1\dots \underline{A}_\ell \dots A_N} = \frac{(-\mathrm{i})^N}{Z^{(0)}(0)} \frac{\delta^N Z^{(1)}}{\delta j_{A_1}\dots \delta k_{A_\ell}\dots\delta j_{A_N}}. \quad (15)$$

The special case of the propagator ($N = 2$ in (14)) yields

$$\begin{aligned}\frac{\partial G_{AB}}{\partial p} &= (-1)^{1+A+B} G^{(1)}_{\underline{A}B} + (-1)^{1+B} G^{(1)}_{A\underline{B}} \\ &= -G^{(1)}_{\underline{A}B} - (-1)^B G^{(1)}_{A\underline{B}}, \end{aligned} \quad (16)$$

where in the second line the fact has been used that in G_{AB} on the l.h.s. A and B are either both commuting or both anticommuting ($\sum_{\nu=1}^{N} A_\nu = 0 \to A + B = 0$).

3 Mass shell, polarizations

All ingredients for the definition of the S-matrix are contained in the Green functions (13). We assume that external lines of the S-matrix element are determined by "physical particles on shell" which are present if the Feynman amplitude for the Fourier transform $\widetilde{G}_{AB}(k)$ of the propagator G_{AB} for a certain value of the four-momentum k at $k^2 - m^2 = \mu \sim 0$ possesses a pole of the type

$$\widetilde{G}_{AB}(k) \underset{\mu\sim 0}{=} \frac{g_{AB}}{Z\mu}, \quad (17)$$

with the sum over spin states yielding the polarization tensor

$$g_{AB} = \sum_{(s)} \overset{(s)}{e}_A \overset{(s)}{e}{}^*_B \quad (18)$$

determined by means of an orthonormalized (finite dimensional) basis

$$\overset{(s)}{e}_A \overset{(t)}{e}{}^*_A = \delta_{(st)} \quad (19)$$

of polarization vectors e_A which is not unique. The transformation

$$\delta \overset{(r)}{e}_A = \delta H_{AB} \overset{(r)}{e}_B \quad (20)$$

with antihermitian $\delta H_{AB} = -\delta H^*_{BA}$ leaves (19) invariant. For instance, for Dirac fermions g_{AB} yields the factor $(\not k + m)$, for gauge bosons the projection operator g_{AB} generically depends on the gauge parameter p.

Of course, (17) may be the result of diagonalizing a mass matrix. It simply means that in the inverse of $\widetilde{G}$, i.e. in the self-energy $\widetilde{\Gamma}_{AB}$ near $\mu \sim 0$ the eigenvectors of $\widetilde{\Gamma}_{AB}$, obeying $\widetilde{\Gamma}_{AB} e_B \sim Z\mu e_A$, are taken as a basis, which spans the degenerate states (spin components) for a certain $\mu \sim 0$. We note that in any case for the regularized theory the new parameter m^2 in μ at this point of our argument may still contain constant (but gauge-dependent) contributions from higher order graphs (in a perturbative expansion, as well as from a nonperturbative point of view). To ease notation in the following we will assume that $e_A = e^*_A$ is real for the physical states and thus δH_{AB} in (20) is antisymmetric. The argument does not change for complex eigenvectors e_A. We also for simplicity from now on assume that the external lines in $G_{A_1\dots A_N}$ do not contain fermions.

Amputating the propagator $G^{(0)}_{AB} = G_{AB}$ from the j-lines (now with grading $A = B = 0$) on the r.h.s. of (16) yields with the amputated "rest" Y from a $G^{(1)}_{\underline{A}B}$, respectively $G^{(1)}_{A\underline{B}}$,

$$\frac{\partial G_{AB}}{\partial p} = -Y_{\underline{A}C} G_{CB} - G_{AC} Y_{C\underline{B}}. \quad (21)$$

Near $\mu \sim 0$ after Fourier transformation ($G \to \widetilde{G}, \widetilde{Y}|_{\mu=0} \to y$) this relation becomes

$$\frac{\partial}{\partial p}\left(\frac{g_{AB}}{Z\mu}\right) = -y_{\underline{A}C} \frac{g_{CB}}{Z\mu} - \frac{g_{AC}}{Z\mu} y_{C\underline{B}}. \quad (22)$$

As usual in such arguments in this step we have made the assumption that the mass shell $\mu = 0$ is not accidentally degenerate with, say, the (gauge-dependent) mass shell of a Higgs ghost (as in the 't Hooft gauge in tree approximation) or of a FP ghost.

The absence of a second order pole μ^{-2} on the r.h.s. of (22) implies the gauge independence $\partial\mu/\partial p = 0$ of μ and hence of the mass parameter m^2. The terms of $\mathcal{O}(\mu^{-1})$ lead to the relation

$$X_{AB} = -X_{BA}, \quad (23)$$

$$X_{AB} = \sum_{(r)} \left(\frac{\overset{(r)}{e}_A}{2Z} \frac{\partial Z}{\partial p} - y_{\underline{A}C} \overset{(r)}{e}_C - \frac{\partial \overset{(r)}{e}_A}{\partial p} \right) \overset{(r)}{e}_B. \quad (24)$$

4 S-matrix

The S-matrix element for N physical external particles (on shell in the sense of (17)) is obtained from the Fourier transform $\widetilde{G}_{A_1\dots A_N}$ of the Green function (13) after amputation of the propagators in each external line, multiplying each line with its proper polarization vector $\overset{(s_i)}{e}_{A_i}$ with spin state (s_i). Furthermore the external lines acquire a renormalization factor $Z_i^{1/2}$. Taking the mass-shell limit $\mu_i = k_i^2 - m_i^2 \to 0$ yields

$$S = \prod_{i=1}^{N} \lim_{\mu_i \to 0} \left[\mu_i \sqrt{Z_i} \overset{(s_i)}{e}_{A_i} \right] \widetilde{G}_{A_1 \dots A_N} . \tag{25}$$

An overall factor like $\prod_i \left[(2\pi)^3 2(m_i^2 + \boldsymbol{k}_i^2)\right]^{-1/2}$ from the external lines is irrelevant (cf. the gauge independence of m_i!) and has been dropped. Differentiation of S with respect to p leads to

$$\frac{\partial S}{\partial p} = \prod_{i=1}^{N} \lim_{\mu_i \to 0} \left[\mu_i \sqrt{Z_i} \right] \sum_{\ell=1}^{N} (A_\ell + B_\ell + C_\ell), \tag{26}$$

where

$$A_\ell = \frac{1}{2Z_\ell} \frac{\partial Z_\ell}{\partial p} \overset{(s_1)}{e}_{A_1} \dots \overset{(s_N)}{e}_{A_N} \widetilde{G}_{A_1 \dots A_N} , \tag{27}$$

$$B_\ell = \overset{(s_1)}{e}_{A_1} \dots \frac{\partial \overset{(s_\ell)}{e}_{A_\ell}}{\partial p} \dots \overset{(s_N)}{e}_{A_N} \widetilde{G}_{A_1 \dots A_N} , \tag{28}$$

$$C_\ell = - \overset{(s_1)}{e}_{A_1} \dots \overset{(s_N)}{e}_{A_N} \dots G^{(1)}_{A_1 \dots \underline{A}_\ell \dots A_N} . \tag{29}$$

Here $\partial \mu / \partial p = 0$, and in C_ℓ (14) for $\partial \widetilde{G} / \partial p$ (in our simplified case with commuting $A_1 \dots A_N$) has been used. In the limit $\mu_i \to 0$ the amputation of the relevant propagator terms (17) at all external lines in $\widetilde{G}_{A_1 \dots A_N}$ in A_ℓ of (27) yields

$$A_\ell = \frac{1}{2Z_\ell} \frac{\partial Z_\ell}{\partial p} \widetilde{G}^{\text{amp}}_{A_1 \dots A_N} \overset{(s_1)}{e}_{A_1} \dots \overset{(s_N)}{e}_{A_N} \prod_{i=1}^{N} \frac{1}{\mu_i Z_i} , \tag{30}$$

where the orthogonality relation (19) has been used. In B_ℓ of (28) the same procedure works for all lines, except for the one with factor $\partial e_{A_\ell} / \partial p$. In the latter we shift the derivative from $\overset{(s_\ell)}{e}_{A_\ell}$ to the propagator factor by (cf. the action of $\partial / \partial p$ on (19))

$$\frac{\partial \overset{(s_\ell)}{e}_{A_\ell}}{\partial p} \frac{\overset{(r)}{e}_{A_\ell} \overset{(r)}{e}_{B_\ell}}{\mu_\ell Z_\ell} = - \overset{(s_\ell)}{e}_{A_\ell} \frac{\partial \overset{(r)}{e}_{A_\ell}}{\partial p} \frac{\overset{(r)}{e}_{B_\ell}}{\mu_\ell Z_\ell} . \tag{31}$$

Finally the analogous amputation at the poles of the propagators in (29) at the line with external source $k_{\underline{A}_\ell}$ produces a factor with y as defined in (22):

$$C_\ell = - \prod_{i=1}^{N} \left(\frac{1}{\mu_i Z_i} \right) \overset{(s_1)}{e}_{A_1} \overset{(s_1)}{e}_{B_1} \dots$$
$$\dots \overset{(s_\ell)}{y}_{\underline{A}_\ell C_\ell} \overset{(r)}{e}_{C_\ell} \overset{(r)}{e}_{B_\ell} \dots \overset{(s_N)}{e}_{A_N} \overset{(s_N)}{e}_{B_N} \widetilde{G}^{\text{amp}}_{B_1 \dots B_N} . \tag{32}$$

Double spin indices $(s_i), (r)$ are being summed everywhere. It should be emphasized that in this way the $G^{(1)}$ amplitude reduces to its pole contribution $\overset{(\ell)}{y}$ and that (32) (as (26) and (28)) becomes proportional to the same amputated ordinary Green function $\widetilde{G}^{\text{amp}}_{A_1 \dots \dots A_N}$. If we formally extract the special factor $\overset{(s_\ell)}{e}_{B_\ell}$ also in (27) by

$$\widetilde{G}^{\text{amp}}_{A_1 \dots A_N} \overset{(s_1)}{e}_{A_1} \dots \overset{(s_N)}{e}_{A_N}$$
$$= \widetilde{G}^{\text{amp}}_{A_1 \dots B_\ell \dots A_N} \overset{(r)}{e}_{B_\ell} \overset{(r)}{e}_{A_\ell} \dots \overset{(s_N)}{e}_{A_N} , \tag{33}$$

adding the contributions (27), (28) and (29) one finds that $\overset{(r)}{e}_{B_\ell}$ is multiplied just by the expression $\overset{(\ell)}{X}_{A_\ell B_\ell}$, as introduced in (23), applied to the line A_ℓ. Apart from that the factors μ_i cancel so that the limit in (25) is a finite (nonvanishing) term proportional to $\Pi_i Z_i^{-1/2}$. Collecting in the sum of (26) the expressions resulting in this manner from (27) with (32), (28) and (32), the *variation* of the S-matrix element with respect to δp has the structure $\delta_1 S \propto \dots \sum_\ell \dots (X_{A_l B_l} \delta p) e_{B_\ell}$. So far the basis e_A has not been changed by varying p. If we take advantage of the freedom to redefine $\overset{(r)}{e}_A$ according to (20) such that $\delta_2 S \propto \dots \sum_\ell \dots (\delta H_{A_\ell B_\ell}) e_{B_\ell}$ with the (antisymmetric) δH adjusted by the (antisymmetric!) X_{AB} to $\delta H_{AB} = -X_{AB} \delta p$, we arrive at $(\delta_1 + \delta_2) S = \delta S = 0$, i.e. at the gauge independence of the S-matrix. For complex e_A antisymmetry of δH_{AB} and X_{AB} is simply replaced by antihermiticity. Fermionic external lines just introduce a few minus signs.

5 Conclusion

The gauge-parameter independence of the S-matrix requires a redefinition of the basis of polarization vectors attached to the external legs of the amputated Green function. Our proof is inherently nonperturbative. It refers to the regularized, but not renormalized amplitude. Therefore, it even applies to any finite perturbative order also for a nonrenormalizable theory. This seems important, because (even renormalizable) gauge theories at low energies may be part of a larger theory (e.g. string theory), where higher modes have been "integrated out" in the low energy regime, yielding effective couplings with (large) negative mass dimension. Our argument was based upon a gauge theory which, following the canonical procedure through extended Hamiltonian and gauge-fixing fermion [19] after integration of certain ghost fields and momenta etc. yields the path integral (2). We did not have to specify the gauge-fixing term further than to be BRS exact. Therefore, a wide class of gauge theories is covered as well, with more complicated ghost interactions than the ones in nonabelian gauge theories [3] based upon Lie groups. Our direct approach completely avoids proceeding through the gauge dependence of 1pi vertices, required in proofs [6] which use Nielsen identities [7]. Especially for an S-matrix element with an arbitrary number of external legs, a proof based upon identities for 1pi vertices would appear very cumbersome.

As we work at the level of a regularized, but not yet renormalized S-matrix element, we are also not forced to deal with possibly delicate questions resulting from the gauge-parameter dependence of counterterms.

A key point in the derivation of the basic identity (11) for Green functions has been the gauge invariance of the measure in (8). Hence a deeper analysis would be required for a theory where no such measure is available. It may be conjectured that a theory, where the renormalizability is caused by an anomaly may be outside the range of applicability of the present proof. Nevertheless, the present line of argument presumably is also useful in that context to exhibit an eventual gauge dependence (and hence unphysicality) of the S-matrix.

All questions regarding the gauge independence with external zero mass particles have been avoided by assuming (wherever necessary) some spontaneous symmetry breaking which provides a suitable regularization without destroying gauge invariance. Clearly the consideration of strictly mass-less external particles within the Bloch–Nordsieck or Lee–Nauenberg [20] mechanism deserves further study, possibly employing again some aspects of the technique described here.

A final remark concerns the possible extension of the present argument to S-matrix elements with strongly interacting external particles (hadrons). Probably also here a proof, generalizing the one known so far only for the axial gauge in nonabelian gauge theories [21] seems to be conceivable.

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