S-matrix elements for gauge theories with and without implemented constraints

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Abstract

We derive an expression for the relation between two scattering transition amplitudes which reflect the same dynamics, but which differ in the description of their initial and final state vectors. In one version, the incident and scattered states are elements of a perturbative Fock space, and solve the eigenvalue problem for the ‘free’ part of the Hamiltonian — the part that remains after the interactions between particle excitations have been ‘switched off’. Alternatively, the incident and scattered states may be coherent states that are transforms of these Fock states. In earlier work, we reported on the scattering amplitudes for QED, in which a unitary transformation relates perturbative and non-perturbative sets of incident and scattered states. In this work, we generalize this earlier result to the case of transformations that are not necessarily unitary and that may not have unique inverses. We discuss the implication of this relationship for Abelian and non-Abelian gauge theories in which the ‘transformed’, non-perturbative states implement constraints, such as Gauss’s law.

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I. INTRODUCTION

Gauge theories always require the imposition of constraints — Euler-Lagrange equations without time derivatives (such as Gauss’s law) are an example. However, when Feynman rules are used, perturbative S-matrix elements are evaluated with incident and scattered (‘in’ and ‘out’) states that do not implement these constraints. In particular, in QED, Gauss’s law, which couples the longitudinal component of the gauge field to charges, is ignored without introducing any errors into S-matrix elements. More generally, the use of ‘wrong’ descriptions of incident and scattered states extends well beyond the failure to implement constraints. S-matrix elements almost never are evaluated between the exact one-particle solutions of the dynamical equations that define even simple models — most gauge theories are far too complicated to permit that. We therefore need to understand the circumstances that allow us to dispense with the imposition of constraints, as well as with the accurate representation of other features of incident and scattered states, in evaluating S-matrix elements.

In previous work we gave a proof that Gauss’s law does not need to be implemented in calculating S-matrix elements for QED or for other Abelian gauge theories [1–4]. The essential idea underlying this proof is that Gauss’s law for QED is unitarily equivalent to the form that it would take for the interaction-free gauge theory, in which the charged sources are decoupled from the gauge field. We know, however, that in the case of non-Abelian gauge theories, Gauss’s law and its limiting form, in which the coupling constant that appears in the covariant derivative has been ‘shut off’, can not be unitarily equivalent [5]. In recent work, we have constructed states that implement Gauss’s law for Yang-Mills theory and QCD [6,7], and have observed that these states can be represented as transforms of ordinary perturbative Fock states, but with a transformation operator that is not unitary and that cannot even be assumed to be non-singular. It therefore becomes important to extend our earlier proof. We now desire a more general result, that relates S-matrix elements between incident and scattered Fock states to the corresponding S-matrix elements for the identical dynamical theory, evaluated for states that are transforms of these Fock states. But in this case — in contrast to Refs. [1–4] — these transforms will not be assumed to be unitary, nor even to have unique inverses.

II. TRANSITION AMPLITUDES FOR PERTURBATIVE AND NONPERTURBATIVE STATES.

We will assume a theory governed by a Hamiltonian \( H \) that can be represented as

\[
H = H_0 + H_1,
\]

where \( H_0 \) describes a ‘free field’ theory, and has a spectrum of perturbative eigenstates \( |n\rangle \) which we will assume to be elements of a Fock space; \( H_1 \) is the part of the Hamiltonian that describes interactions among the particle excitations which, in general, will include ghost excitation modes. In particular, we will apply this formalism to gauge theories in which \( H_0 \) describes noninteracting charged particles (we will understand ‘charge’ to include electrical charge, color charge, etc.) and excitations of gauge fields; and \( H_1 \) describes the interactions
— all those parts of $H$ that vanish when the coupling constant characteristic of this gauge theory is set = 0. We will assume that the incident and scattered states of this theory are to be represented as a set of nonperturbative eigenstates $|\bar{n}\rangle$, of the form

$$|\bar{n}\rangle = \Xi |n\rangle.$$  \tag{2.2}$$

where $\Xi$ is an operator which we will neither assume to be unitary, nor even to have a unique inverse. This will enable us to apply the work reported in this paper to gauge theories in which the state $|n\rangle$ represents a perturbative state in non-Abelian gauge theories (for example, a state consisting of gluons and quarks) and $|\bar{n}\rangle$ represents the corresponding state that implements the non-Abelian Gauss’s law. An explicit construction of a transformation operator $\Xi$ for Yang-Mills theory and QCD has recently been given [6, 7].

We will specify two scattering states based on these two alternative descriptions of incident particle states — the perturbative Fock state $|i\rangle$, which obeys $(H_0 - E_i)|i\rangle = 0$, and the nonperturbative state $|\bar{i}\rangle = \Xi |i\rangle$. These two scattering states are given by

$$|\varphi_i\rangle = \left[1 + \left(E_i - H + i\epsilon\right)^{-1}H_1\right]|i\rangle$$  \tag{2.3}$$

and

$$|\bar{\varphi}_i\rangle = \left[1 + \left(E_i - H + i\epsilon\right)^{-1}(H - E_i)\right]\Xi |i\rangle$$  \tag{2.4}$$

respectively. Our purpose in this work is to find a relation between the transition amplitudes

$$T_{f,i} = \langle f | H_1 | \varphi_i \rangle,$$  \tag{2.5}$$

and

$$\bar{T}_{f,i} = \langle \bar{f} | (H - E_f) | \bar{\varphi}_i \rangle.$$  \tag{2.6}$$

We proceed by defining another Hamiltonian, $\bar{H}$, by

$$\bar{H} = \Xi^\dagger H \Xi = \bar{H}.$$  \tag{2.7}$$

When $\Xi$ is unitary, it is easy to shift $\Xi$ or $\Xi^\dagger$ from one side of Eq. (2.7) to the other. But when $\Xi$ is not unitary, we need to define additional auxiliary quantities to achieve that objective. We define

$$\Xi \Xi^\dagger = \alpha = \alpha^\dagger.$$  \tag{2.8}$$

and $\mathcal{A}$ and $\mathcal{A}^\dagger$ by

$$\mathcal{A}\alpha = 1 \quad \text{and} \quad \alpha\mathcal{A}^\dagger = 1.$$  \tag{2.9}$$

We assume that $\mathcal{A}$ and $\mathcal{A}^\dagger$ exist, but not that $\mathcal{A} = \mathcal{A}^\dagger$, allowing for the possibility that $\alpha$ may not have a unique inverse. We also define

$$\mathcal{X} = \Xi^\dagger \mathcal{A}^\dagger \Xi = \mathcal{X}^\dagger.$$  \tag{2.10}$$

With this expanded set of operators, we easily obtain
\[ \Xi \mathcal{X} = \left[ (\Xi \Xi^\dagger) A^\dagger \right] A \Xi = A \Xi \]  

(2.11)

and its hermitian adjoint
\[ \mathcal{X} \Xi^\dagger = \Xi^\dagger A^\dagger. \]  

(2.12)

And, by multiplying Eq. (2.7) by \( A \Xi \) on the left and using Eq. (2.11),
\[ H \Xi = A \Xi \bar{H} = \Xi \mathcal{X} \bar{H}. \]  

(2.13)

We can transform Eq. (2.4) by using Eq. (2.13) to shift \( \Xi \) to the extreme left, systematically replacing \( H \) by \( \mathcal{X} \bar{H} \) in the wake of the shifted \( \Xi \). This can be seen clearly from the representation of \( (E_i - H + i\epsilon)^{-1} \Xi \) as
\[ \left\{ 1 + \frac{H}{E_i^{(+)}} + \frac{H}{E_i^{(+)}} \cdot \frac{H}{E_i^{(+)}} \cdots + (\frac{H}{E_i^{(+)}})^n \cdots \right\} \left( \frac{\Xi}{E_i^{(+)}} \right) = \]  

(2.14)

\[ \left( \frac{\Xi}{E_i^{(+)}} \right) \left\{ 1 + \frac{\mathcal{X} \bar{H}}{E_i^{(+)}} + \frac{\mathcal{X} \bar{H}}{E_i^{(+)}} \cdot \frac{\mathcal{X} \bar{H}}{E_i^{(+)}} \cdots + (\frac{\mathcal{X} \bar{H}}{E_i^{(+)}})^n \cdots \right\} \]

(where \( E_i^{(+)} = E_i + i\epsilon \)), which illustrates the movement of \( \Xi \) to the left, transforming Eq. (2.4) into
\[ |\bar{\varphi}_i \rangle = \Xi \left[ 1 + (E_i - \mathcal{X} \bar{H} + i\epsilon)^{-1} (\mathcal{X} \bar{H} - E_i) \right] |i \rangle. \]  

(2.15)

Furthermore, in Eq. (2.13), we can set \( \bar{H} = H_0 + \bar{H}_1 \) and \( \Xi \mathcal{X} \bar{H}_1 = \bar{H}_1 - (1 - \Xi \mathcal{X}) \bar{H}_1 \), and obtain
\[ \bar{H}_1 = H_1 \Xi + H_0 \Xi - \Xi \mathcal{X} H_0 + (1 - \Xi \mathcal{X}) \bar{H}_1. \]  

(2.16)

Adding and subtracting \( H_0 \) from the right hand side of Eq. (2.16) leads to
\[ \bar{H}_1 = H_1 \Xi - H_0 (1 - \Xi) + (1 - \Xi \mathcal{X}) \bar{H}; \]  

(2.17)

and, after multiplying the hermitian adjoint of Eq. (2.17) by \( \mathcal{X} \) on the left and using Eq. (2.11) to transform the resulting equation, we obtain
\[ \mathcal{X} \bar{H}_1 = \Xi^\dagger A^\dagger H_1 + (1 - \mathcal{X}) H_0 - \left( 1 - \Xi^\dagger A^\dagger \right) H_0 + \mathcal{X} \bar{H} \left( 1 - \Xi^\dagger A^\dagger \right). \]  

(2.18)

We can now use Eq. (2.18) to obtain
\[ (\mathcal{X} \bar{H} - E_i) |i \rangle = \left[ \Xi^\dagger A^\dagger H_1 + \left( \mathcal{X} \bar{H} - E_i \right) \left( 1 - \Xi^\dagger A^\dagger \right) \right] |i \rangle. \]  

(2.19)

We substitute Eq. (2.19) into Eq. (2.13); and, in the resulting expression, systematically use \( \mathcal{X} \bar{H} \Xi^\dagger = \Xi^\dagger A^\dagger H_0 \) to shift \( \Xi^\dagger \) to the left in the same manner as in Eq. (2.14), to obtain
\[ |\bar{\varphi}_i \rangle = |i \rangle + \alpha \left( E_i - A^\dagger H_0 + i\epsilon \right)^{-1} A^\dagger H_1 |i \rangle + i\epsilon \Xi \left( E_i - \mathcal{X} \bar{H} + i\epsilon \right)^{-1} \left( 1 - \Xi^\dagger A^\dagger \right) |i \rangle. \]  

(2.20)
Since $\alpha A^\dagger = 1$, it is easy to see that
\[(E_i - A^\dagger H \alpha + i\epsilon)^{-1} A^\dagger = A^\dagger (E_i - H + i\epsilon)^{-1};\] (2.21)
and similarly, we observe that
\[\Xi (E_i - X^\dagger \bar{H} + i\epsilon)^{-1} (1 - \Xi^\dagger A^\dagger) = (E_i - H + i\epsilon)^{-1} (\Xi - 1)\] (2.22)
follows from Eq. (2.13). These two identities can be used to rewrite Eq. (2.20) as
\[|\bar{\phi}_i\rangle = \left[1 + (E_i - H + i\epsilon)^{-1} H_0 + H (1 - \Xi)\right] |\phi_i\rangle + \epsilon (E_i - H + i\epsilon)^{-1} (\Xi - 1) |\phi_i\rangle.\] (2.23)

We now use Eq. (2.13) to rewrite Eq. (2.6) as
\[\bar{T}_{f,i} = (f | (\bar{H}X - E_f) \Xi | \bar{\phi}_i\rangle,\] (2.24)
as well as to obtain the identity
\[H_1 = \Xi X \bar{H}_1 - (1 - \Xi X) H_0 + H (1 - \Xi)\] (2.25)
and its adjoint
\[H_1 = \bar{H}_1 \Xi - H_0 (1 - \Xi \Xi^\dagger) + (1 - \Xi^\dagger) H.\] (2.26)
Finally, we use Eqs. (2.23) and (2.26) to transform Eq. (2.24) into
\[\bar{T}_{f,i} = T_{f,i} + (E_i - E_f) \langle f | (\Xi^\dagger - 1) \left[|\varphi_i\rangle + \epsilon (E_i - H + i\epsilon)^{-1} (\Xi - 1) |i\rangle\right]\] (2.27)
+ $i\epsilon \langle f | \left[(\Xi^\dagger - 1) (E_i - H + i\epsilon)^{-1} H_1 + H_1 (E_i - H + i\epsilon)^{-1} (\Xi - 1) \right]|i\rangle$
- $i\epsilon \langle f | \left((\Xi^\dagger - 1) (\Xi - 1) |i\rangle + \epsilon^2 \langle f | \left[(\Xi^\dagger - 1) (E_i - H + i\epsilon)^{-1} (\Xi - 1) \right] |i\rangle$
where $|\varphi_i\rangle$ is given by Eq. (2.3).

III. DISCUSSION.

When $\Xi$ is unitary, $\alpha = 1$, $A = A^\dagger = 1$, and $X = 1$. The expression in Refs. [2–4] that relates $T_{f,i}$ and $\bar{T}_{f,i}$ for a unitary transformation, $\Xi_{\text{unit}}$, is given by
\[T_{f,i} = T_{f,i} + (E_i - E_f) \langle f | (\Xi_{\text{unit}}^\dagger - 1) |\varphi_i\rangle\] (3.1)
+ $i\epsilon \langle f | \left[(\Xi_{\text{unit}}^\dagger - 1) (E_i - H + i\epsilon)^{-1} H_1 - \bar{H}_1 (E_i - \bar{H} + i\epsilon)^{-1} (\Xi_{\text{unit}}^\dagger - 1) \right]|i\rangle$.\)
When $\Xi$ is the unitary transformation $\Xi_{\text{unit}}$, it is straightforward to transform Eq. (3.1) so that its form is identical to Eq. (2.27). The converse does not hold, however. Eq. (3.1) does not describe the relation between $T_{f,i}$ and $\bar{T}_{f,i}$ correctly when $\Xi$ is not unitary; auxiliary quantities — $\alpha$, $A$, $A^\dagger$, and $X$ — would be required to avoid quadratic $\epsilon$ terms by using barred as well as unbarred Hamiltonians in an equation that resembles Eq. (3.1).
It is somewhat surprising that the relation between $T_{f,i}$ and $\tilde{T}_{f,i}$ is so robust, that such a general transformation — one that is neither required to be unitary nor even to have a unique inverse — makes no significant changes in Eq. (2.27). This robustness may well account for our freedom to describe charged particle states quite imperfectly in evaluating perturbative S-matrix elements in gauge theories. When we use Feynman rules in QED in covariant gauges, we fail to account for the electrostatic field that is required by Gauss’s law to accompany the incident and scattered charged particles. Moreover, we similarly omit the ‘dressing’ by transversely polarized propagating photons, which account for the magnetic field of a moving charged particle. Nevertheless, the resulting S-matrix elements suffer no harm, save for the infrared divergences which stem from the absence of the transversely polarized ‘soft’ photons from the charged particle state, and which are curable by the Block-Nordsieck algorithm [4]. It is not certain, however, that the immunity that applies in QED when we fail to implement Gauss’s law [1,1] — namely, that except for the expressions for the renormalization constants, S-matrix elements are unchanged when $T_{f,i}$ is substituted for $\tilde{T}_{f,i}$ — also applies to QCD.

The following remarks apply to the relation between $\tilde{T}_{f,i}$ and $T_{f,i}$ described by Eq. (2.27):
The term in Eq. (2.27) that is proportional to $(E_i - E_f)$ clearly vanishes in the S-matrix, which is proportional to $\delta(E_i - E_f)$. The terms in Eq. (2.27) that are proportional to $i\epsilon$ or $(i\epsilon)^2$, vanish as $\epsilon \rightarrow 0$, unless $(i\epsilon)^{-1}$ or $(i\epsilon)^{-2}$ appears in a matrix element that has $i\epsilon$ or $(i\epsilon)^2$ respectively as a coefficient. There are various situations in which inverse powers of epsilon can arise in these matrix elements. In one case, the matrix element $\langle n | (\Xi - 1) | i \rangle$ develops delta-function singularities of the form

$$\langle n | (\Xi - 1) | i \rangle = \xi(E_n)\delta(E_n - E_i) + \text{less singular or non-singular terms},$$

where $\xi(E_n)$ is a relatively smooth function of $E_n$. An instructive example of $i\epsilon$ singularities of this variety is the transition amplitude that describes nonrelativistic particles scattered by a non-isotropic potential represented by $H_1$. In this example we will choose $\Xi$ to be the unitary rotation operator $R$, which rotates the non-isotropic potential through some set of finite Eulerian angles, so that $R$ will commute with $H_0$ but not with $H_1$. In this case $\tilde{T}_{f,i}$ is not — and should not be — identical to $T_{f,i}$, since the former will describe a situation in which the non-isotropic potential has been rotated, but the incident and scattered states acted on by this potential have remained fixed in space. The Green function $(E_i - H + i\epsilon)^{-1}$ in Eq. (2.27) can be expanded in the form

$$(E_i - H + i\epsilon)^{-1} = (E_i - H_0 + i\epsilon)^{-1} + (E_i - H_0 + i\epsilon)^{-1}H_1(E_i - H + i\epsilon)^{-1},$$

and the propagator $(E_i - H_0 + i\epsilon)^{-1}$ is free to commute with $(R - 1)$ and $(R^\dagger - 1)$ and to act directly on $|i\rangle$ and $\langle f |$, producing inverse powers of $i\epsilon$. We find, in this case, that

$$\langle f | (R^\dagger - 1)(E_i - H + i\epsilon)^{-1}H_1|i\rangle = (i\epsilon)^{-1}\langle f | (R^\dagger - 1)T|i\rangle,$$

where $T = H_1 + H_1(E_i - H + i\epsilon)^{-1}H_1$,

$$\langle f | H_1(E_i - H + i\epsilon)^{-1}(R - 1)|i\rangle = (i\epsilon)^{-1}\langle f | T(R - 1)|i\rangle,$$
\[
\langle f \mid \left( R^\dagger - 1 \right) (E_i - H + i \epsilon)^{-1} (R - 1) \mid i \rangle = (i \epsilon)^{-2} \left[ \langle f \mid \left( R^\dagger - 1 \right) T (R - 1) \mid i \rangle + \mathcal{O}(\epsilon) \right],
\]

so that Eq. (2.27) for this case, in the limit \( E_f \to E_i \) and \( \epsilon \to 0 \), does not describe any relationship between \( T_{f,i} \) and \( T^\dagger_{f,i} \), but reduces to the trivial identity

\[
T_{f,i} = T^\dagger_{f,i} - T_{f,i}.
\]

Eq. (2.27) can, however, provide useful information about the relation between \( T^\dagger_{f,i} \) and \( T_{f,i} \) in QED, when \( \Xi_{\text{unit}} \) is the operator that transforms the charged perturbative Fock states into states that implement Gauss’s law. The unitary operator \( \Xi_{\text{unit}} \) that is used in implementing Gauss’s law in QED has the form \( \Xi_{\text{unit}} = e^D \), where \( D \) is given in earlier work [1–4]. And \( (e^D - 1) \) is a power series in \( D \); neither \( D \) nor \( D^n \), for any value of \( n \), can stand alone in matrix elements between perturbative Fock states that describe propagating observable particles — photons or electrons. Nor does \( [\exp (D) - 1] \) commute with \( H_0 \); \( (\tilde{T}_{f,i} - T_{f,i}) \) therefore can not have the kind of delta-function singularities, in this case, that deprive Eq. (2.27) of all useful content when a unitary transform \( \Xi_{\text{unit}} \) commutes with \( H_0 \). Inverse powers of \( i \epsilon \) do arise when Eq. (2.27) is applied to QED, but they arise in a very limited way, and do not invalidate the conclusion that \( T^\dagger_{f,i} \) and \( T_{f,i} \) are identical, although that identity obtains only after changes are made in renormalization constants to reflect the fact that \( (\Xi_{\text{unit}} - 1) \) and \( (\Xi_{\text{unit}}^\dagger - 1) \) combine with \( H_1 \) to produce additional self-energy insertions in external charged particle lines. These additional self-energy insertions change the expressions for renormalization constants but do not have any further effect on \( S \)-matrix elements [1–4].

The features of the unitary transformation operator, \( \Xi_{\text{unit}} = e^D \) that is applied to the implementation of Gauss’s law in QED limits the appearance of inverse powers of \( i \epsilon \) in matrix elements in Eqs. (2.27) or (3.1), so that only renormalization constants are affected by the substitution of \( T^\dagger_{f,i} \) for \( T_{f,i} \). But it is uncertain to what extent this immunity from substantial, physically observable differences between \( T^\dagger_{f,i} \) and \( T_{f,i} \) extends to the transition amplitude in QCD obtained with the non-unitary \( \Xi \) that implements the non-Abelian Gauss’s law. We will not pursue this question further here, but will leave the detailed application of Eq. (2.27) to the \( S \)-matrix in QCD for a later work.

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