Finite S matrix

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When massless particles are involved, the traditional scattering matrix (*S* matrix) does not exist: It has no rigorous nonperturbative definition and has infrared divergences in its perturbative expansion. The problem can be traced to the impossibility of isolating single-particle states at asymptotic times. On the other hand, the troublesome nonseparable interactions are often universal: In gauge theories, they factorize so that the asymptotic evolution is independent of the hard scattering. Exploiting this factorization property, we show how a finite "hard" *S* matrix, S_H , can be defined by replacing the free Hamiltonian with a soft-collinear asymptotic Hamiltonian. The elements of S_H are gauge invariant and infrared finite and exist even in conformal field theories. One can interpret elements of S_H alternatively 1) as elements of the traditional *S* matrix between dressed states, 2) as Wilson coefficients, or 3) as remainder functions. These multiple interpretations provide different insights into the rich structure of S_H .

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One of the most fundamental objects in high energy physics is the scattering or S matrix. Not only is it a bridge between a definition of a quantum theory and data from particle colliders, but the study of the S matrix itself has led to deep insights into the mathematical and physical pillars of quantum field theory itself. The idea behind the S matrix is that it gives the amplitude for a set of particles in an "in" state $|\psi_{in}\rangle$ at $t = -\infty$ to turn into a different set of particles in an "out" state $\langle \psi_{out} |$ at $t = +\infty$. To go from this intuitive picture to a mathematically rigorous definition of the S matrix has proven remarkably challenging. For example, suppose we take the in and out states to be eigenstates of the Hamiltonian H with energy E. Then they would evolve in time only by a phase rotation, and the S-matrix elements would all have the form $\lim_{t\to\infty} e^{-2iEt} \langle \psi_{out} | \psi_{in} \rangle$. Such an *S* matrix would be both ill defined (because of the limit) and trivial (because of the projection). In nonrelativistic quantum mechanics, one avoids this infinitely oscillating phase by subtracting from H the free Hamiltonian $H_0 = \frac{\vec{p}^2}{2m}$. More precisely, one looks for states $|\psi\rangle$ which, when evolved with the full Hamiltonian, agree with in and out states evolved with the free Hamiltonian: $e^{-iHt}|\psi\rangle \rightarrow e^{-iH_0t}|\psi_{in}\rangle$ as $t \to -\infty$ and $e^{-iHt} |\psi\rangle \to e^{-iH_0 t} |\psi_{out}\rangle$ as $t \to +\infty$. Then the projection of in states onto out states is given by matrix

^{*}holmfridur_hannesdottir@g.harvard.edu [†]schwartz@g.harvard.edu elements $\langle \psi_{\text{out}} | S | \psi_{\text{in}} \rangle$ of the operator $S = \Omega_{+}^{\dagger} \Omega_{-}$ where the Møller operators are defined as $\Omega_{\pm} = e^{iHt_{\pm}} e^{-iH_0t_{\pm}}$, with t_{\pm} shorthand for the $t \to \pm \infty$ limit. In this way, the free evolution, which is responsible for the infinite phase, is removed. Note that $\lim_{t\to\pm\infty} e^{-iHt} | \psi \rangle$ is not a well-defined state, so the in and out states should be thought of as either Heisenberg picture states or as Schrödinger picture states at t = 0 not at $t = \pm \infty$ (see Fig. 1). Defining the *S* matrix this way gives sensible results and a pleasing physical picture: Particles we scatter are free when not interacting. Their freedom means they should have momentum defined by the free Hamiltonian, and the *S* matrix encodes the effects of interactions impinging on this freedom.

In quantum field theory, a similar construction is fraught with complications. The Møller operators, which convert from the Heisenberg picture to the interaction picture, do not exist as unitary operators acting on a Fock space (Haag's theorem [1]). So one must work entirely in the Heisenberg picture without reference to H_0 . The matching of the states at $t \to \pm \infty$ is then replaced with an asymptotic condition on the matrix elements of fields. In the Haag-Ruelle construction [2–4], a mass gap is required to isolate the few-particle asymptotic states as limits of carefully constructed wave packets. From there, one can derive the Lehmann-Symanzik-Zimmermann (LSZ) reduction theorem, relating elements of the *S* matrix to time-ordered products of fields [5,6].

While it is satisfying to know that the *S* matrix can be rigorously defined, its existence requires a theory with a mass gap, a unique vacuum state, and fields whose two-point functions vanish exponentially at spacelike separation. None of these requirements hold in any real-world theory. The practical resolution to this impasse is to ignore Haag's

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FIG. 1. (Left) The traditional *S* matrix is computed from Fock states evolved using H_0 and *H*. (Right) The hard *S* matrix is computed either using Fock states evolved with H_{as} and *H* or using dressed states evolved with H_0 and *H*.

theorem, ignore that charged particles cannot be isolated and other assumptions, and simply use the LSZ reduction theorem as if it were true, computing *S*-matrix elements with Feynman diagrams. Although the resulting matrix elements are singular (due to infrared divergences), as long as one combines *S*-matrix elements computed this way into observable cross sections, the singularities will drop out. This is guaranteed by the Kinoshita–Lee–Nauenberg (KLN) theorem [7,8], which says that infrared divergences will cancel when initial and final states are summed over, or by its stronger version, that the cancellation occurs when initial *or* final states are summed over [9]. Despite the success of this pragmatic approach, it remains deeply unsettling that the underlying object we compute, the *S* matrix, has no formal definition even in QED.

There has been intermittent progress on constructing an S matrix for QED (and QCD) over the last 50 or so years. The infrared divergence problem of the S matrix can be seen already in nonrelativistic scattering off a Coulomb potential. Because of its $\frac{1}{r}$ behavior, the Coulomb potential is not square integrable, and the asymptotic states do not exist. This complication was observed by Dollard [10] and resolved by using a modified Hamiltonian $H_{as}(t)$ that appends the dominant large-distance behavior of the Coulomb interaction to the free Hamiltonian. Chung [11], independently, observed that if instead of scattering single-particle Fockstate elements, one scatters linear combinations of these elements, similar to coherent states used in quantum optics (and to an early attempt by Dirac [12]), finite amplitudes would result. In Chung's construction, the IR divergent phase space integrals from cross-section calculations are moved into the definition of the states. Faddeev and Kulish [13] subsequently redefined the S matrix to include the dominant long-distance interactions of QED in its asymptotic Hamiltonian (similar to Dollard), and identified Chung's coherent states as arising during the asymptotic evolution. Over the years, various subtleties in the coherentstate approach to soft singularities in QED have been explored [14–16], and attempts have been made to construct a finite S matrix for theories like QCD with massless charged particles and hence, collinear singularities [17–20].

Remarkably, in all this literature, there are very few explicit calculations of what a finite *S* matrix looks like. Indeed, almost all of the papers concentrate on the singularities alone. Doing so sidesteps the challenge of how to handle finite parts of the amplitudes and precludes the possibility of actually calculating anything physical. With an explicit prescription, you have to contend with questions such as what quantum numbers do the dressed states have? They cannot have well-defined energy and momentum outside of the singular limit, since they are superpositions of states with different numbers of noncollinear finite-energy particles.

The basic aspiration of much of this literature is that when there are long-range interactions, the *S* matrix should be defined through asymptotic Møller operators $\Omega_{\pm}^{as} = e^{iH_{t_{\pm}}}e^{-iH_{as}t_{\pm}}$ with some kind of asymptotic Hamiltonian H_{as} replacing the free Hamiltonian H_0 . Despite the simple summary, working out the details and establishing a productive calculational framework has proved a resilient challenge.

In this paper, we continue the quest for a finite *S* matrix by folding into the previous analysis insights from the modern understanding of scattering amplitudes and factorization. We argue that the principle by which the asymptotic Hamiltonian is to be defined is not that the dominant long-distance interactions be included (which allows for $H_{as} = H$ and S = 1), but that the evolution of the states be independent of how they scatter.

In gauge theories, infrared divergences can be either soft or collinear in origin. Both soft and collinear interactions are universal and can be effectively separated from the remainder of the scattering process. Factorization has been understood from many perspectives [21–29]. A precise statement of factorization can be found in [28,29], where it is proven that the IR divergences of any *S* matrix in QCD are reproduced by the product of a hard factor, collinear factors for each relevant direction, and a single soft factor. A useful language for understanding factorization is softcollinear effective theory (SCET) [23–27,30,31]. The SCET Lagrangian is

$$\mathcal{L}_{\text{SCET}} = -\frac{1}{4} (F_{\mu\nu}^{s})^{2} + \sum_{n} -\frac{1}{4} (F_{\mu\nu}^{c,n})^{2} + \sum_{n} \bar{\psi}_{n}^{c} \frac{\not{n}}{2} \left[in \cdot D + i \not{D}_{c\perp} \frac{1}{i\bar{n} \cdot D_{c}} i \not{D}_{c\perp} \right] \psi_{n}^{c} + \mathcal{L}_{\text{Glauber}}, \qquad (1)$$

where *s* and *c*, *n* are soft and collinear labels, respectively; these act like quantum numbers for the fields. The derivation of the SCET Lagrangian and more details on the notation an be found in the reviews [30,31]. The Glauber interactions denoted by $\mathcal{L}_{\text{Glauber}}$ are discussed in [32]; when they are included, the SCET Lagrangian can reproduce all of the IR singularities of any non-Abelian

gauge theory. The main relevant features of the SCET Lagrangian are that 1) there are no interactions between fields with different collinear-direction labels (up to Glauber effects), and 2) collinear particles going in different directions only interact through soft photons or gluons with eikonal interactions. We define the asymptotic Hamiltonian $H_{\rm as}$ as the SCET Hamiltonian appended with the free Hamiltonians for massive particles, which we denote with $H_{\rm as} = H_{\rm sc}$.

In collider physics applications, one typically adds to the SCET Hamiltonian a set of operators necessary to reproduce the hard scattering of interest. For example, one might add $\Delta \mathcal{H} = C \bar{\psi} \gamma^{\mu} \psi$ for jet physics applications in $e^+ e^$ collisions. Then one determines the Wilson coefficient C by choosing it such that matrix elements computed using SCET agree with matrix elements computed in the full theory. Importantly, the infrared divergences cancel in the difference so that C is IR-finite order by order in perturbation theory. Motivated by such cancellations, we define hard Møller operators as $\Omega^{H}_{\pm} = e^{iHt_{\pm}}e^{-iH_{sc}t_{\pm}}$ and the hard S *matrix* as $S_H = \Omega_+^{H\dagger} \Omega_-^H$. Because H_{sc} reproduces the IRdivergence-generating soft and collinear limits of H, we expect the hard S matrix will be IR finite. In addition, S_H and corresponding observables will inherit the symmetry properties of \mathcal{L}_{SCET} , such as Lorentz invariance, as opposed to when $H_{\rm as}$ includes explicit energy and angular cutoffs.

To evaluate matrix elements of S_H in perturbation theory, one could attempt to work out Feynman rules in an interaction picture based on H_{sc} instead of H_0 . A propagator would then be a Green's function for H_{sc} , which has no known closed-form expression. Alternatively, we can write S_H suggestively as (cf. [13,18])

$$S_H = \Omega_+^{H\dagger} \Omega_-^H = \Omega_+^{\rm sc} \Omega_+^{\dagger} \Omega_- \Omega_-^{\rm sc\dagger}, \qquad (2)$$

where $\Omega^{\rm sc}_{\pm} = e^{iH_0t_{\pm}}e^{-iH_{\rm sc}t_{\pm}}$. This encourages us to define

$$|\psi_{\rm in}^d\rangle = \Omega_{-}^{\rm sc\dagger} |\psi_{\rm in}\rangle$$
 and $|\psi_{\rm out}^d\rangle = \Omega_{+}^{\rm sc\dagger} |\psi_{\rm out}\rangle$ (3)

as dressed in and out states. Then,

$$\langle \psi_{\text{out}} | S_H | \psi_{\text{in}} \rangle = \langle \psi_{\text{out}}^d | S | \psi_{\text{in}}^d \rangle.$$
 (4)

We will take $|\psi_{in}\rangle$ and $|\psi_{out}\rangle$ to be eigenstates of the free momentum operator P_0^{μ} with a few (finite number of) particles in them. Thus, we can think of S_H as computing either projections among few-particle states with the hard Møller operators or projections of dressed states with the original S-matrix Møller operators. For example, in the process $e^+e^- \rightarrow Z$ in QED, $|\psi_{in}\rangle$ would be an e^+e^- state of definite momentum and $|\psi_{in}^{\mu}\rangle$ a superposition of $|e^+e^-\rangle$, $|e^+e^-\gamma\rangle$, $|e^+e^-\gamma\gamma\rangle$, and so on.

More explicitly, we can relate $|\psi_{in}^d\rangle$ to $|\psi_{in}\rangle$ using timeordered perturbation theory (TOPT). For example, if $|\psi_{in}\rangle$ is the state of an electron with momentum \vec{p} , then in QED,

$$\begin{split} |\psi_{\rm in}^d\rangle &= |\bar{u}_s(p)\rangle + e \sum_{\epsilon} \int \frac{d^{d-1}k}{(2\pi)^{d-1}} \\ &\times \frac{1}{2\omega_p} \frac{1}{2\omega_k} \frac{2p \cdot \epsilon}{\omega_k - \frac{\vec{p} \cdot \vec{k}}{\omega_p} - i\epsilon} |\bar{u}_s(p-k), \epsilon(k)\rangle + \cdots . \end{split}$$
(5)

The denominator factor comes from the soft expansion of the TOPT propagator $(\omega_{p-k} + \omega_k - \omega_p - i\varepsilon)^{-1}$. Note that the states in the expansion of $|\psi_{in}^d\rangle$ have different energies. Although electric charge and three-momentum are conserved, energy is not as we evolve with Ω_{-}^{as} in TOPT. Due to the IR-divergent integral over \vec{k} , dressed states do not exist (in contrast to $|\psi_{in}\rangle$ and $|\psi_{out}\rangle$), but they do provide a useful qualitative handle on scattering.

As a concrete example, we now compute S_H for deepinelastic scattering, $e^-\gamma^* \rightarrow e^-$ in QED with massless fermions at momentum transfer $Q = \sqrt{-q^2}$ in the Breit frame. At order e^2 , the loop contribution to the *S*-matrix element is, in $\overline{\text{MS}}$ and $d = 4 - 2\epsilon$ dimensions [33],

$$\mathcal{M}_{A} = \mathcal{M}_{0} \frac{\alpha}{4\pi} \left[\frac{1}{\epsilon_{\rm UV}} - \frac{2}{\epsilon_{\rm IR}^{2}} - \frac{2\ln\frac{\mu^{2}}{Q^{2}} + 4}{\epsilon_{\rm IR}} - \ln^{2}\frac{\mu^{2}}{Q^{2}} - 3\ln\frac{\mu^{2}}{Q^{2}} - 8 + \frac{\pi^{2}}{6} \right]$$
(6)

with \mathcal{M} defined by $S_H = 1 + (2\pi)^4 \delta^4 (q + p_1 - p_2) i \mathcal{M}$ and $\mathcal{M}_0 = -e\bar{u}(p_2)\gamma^{\mu}u(p_1)$ is the tree-level amplitude.

While this S-matrix element is IR divergent, there are other contributions to S_H at the same order. These can be thought of as S-matrix elements for the $e^-\gamma$ components of $|\psi_{in}^d\rangle$ or $|\psi_{out}^d\rangle$. We can represent the new graphs as cuts through a broader graph, going from $0 \rightarrow -\infty \rightarrow \infty \rightarrow 0$. The first and last transitions go backward in time and represent the dressing and undressing of the state in the asymptotic regions. For example, the graph with both photon vertices coming from soft-collinear interaction in H_{sc} is

$$\mathcal{M}_{B} = \mathcal{M}_{0}e^{2}\mu^{4-d}\int \frac{d^{d-1}k}{(2\pi)^{d-1}} \times \frac{1}{2\omega_{k}}\frac{1}{2\omega_{1}}\frac{1}{2\omega_{2}}\frac{8\omega_{1}\omega_{2}}{\omega_{k} - \frac{\vec{p}_{1}\cdot\vec{k}}{\omega_{1}} - i\varepsilon}\frac{1}{\omega_{k} - \frac{\vec{p}_{2}\cdot\vec{k}}{\omega_{2}} - i\varepsilon}$$
(7)

To derive this integrand, we have power expanded in the soft limit as in the method-of-regions approach [34], rather than using $\mathcal{L}_{\text{SCET}}$ directly. Although energy is not conserved in the asymptotic regions, the central region gives $\delta(\omega_k + \omega_{p_1-k} - \omega_k - \omega_{p_2-k}) \cong \delta(\omega_1 - \omega_2)$, which is factored out in the definition of \mathcal{M} .

This integral is scaleless and vanishes. Although we cannot easily separate all the UV and IR poles, the double soft and collinear pole in this amplitude is

$$\mathcal{M}_B = \mathcal{M}_0 \frac{\alpha}{4\pi} \left[-\frac{2}{\epsilon_{\rm IR}^2} + \cdots \right]. \tag{8}$$

Focusing on the double pole also lets us restrict to just the soft graphs, as they contain the complete soft-collinear singularity. There are also graphs with one vertex coming from H_{sc} and one coming from H:

$$\mathcal{M}_C + \mathcal{M}_D = + + (9)$$

$$= \mathcal{M}_0 \frac{\alpha}{4\pi} \bigg[\frac{4}{\epsilon_{\rm IR}^2} + \cdots \bigg]. \tag{10}$$

The double IR pole from the S-matrix element cancels exactly in the sum $\mathcal{M}_A + \mathcal{M}_B + \mathcal{M}_C + \mathcal{M}_D$, as anticipated.

It is worth emphasizing the even the double-pole calculation is not trivial and requires careful manipulation of the distributions involved (cf. Ref. [9]). Moreover, the cancellation is different in nature from the cancellation in the computation of a Wilson coefficient. There, the soft exchange graph (the analog of \mathcal{M}_B) is *subtracted* from \mathcal{M}_A ; here, the graphs add, with the cancellation coming from graphs $\mathcal{M}_C + \mathcal{M}_D$ with one soft and one regular vertex.

The other TOPT diagrams involving soft-collinear vertices in $H_{\rm sc}$, such as

are not infrared divergent. In fact, the second diagram is zero, because there is no electron-positron annihilation vertex in $H_{\rm sc}$. Similarly, there are no diagrams with the hard vertex in the asymptotic regions, as $H_{\rm sc}$ has only soft and collinear interactions.

To see the cancellation of subleading IR poles explicitly, we need regulators other than those provided by dimensional regularization, such as off shellness (see [33,35]), or explicit phase space restrictions. One should also then include graphs involving the collinear interactions in H_{sc} as well as a zero-bin subtraction to avoid overcounting [35]. Using dimensional regularization is simplest, since all of the graphs other than \mathcal{M}_A are scaleless. Thus, after removing UV poles with renormalization, we find

$$\langle e^{-}|S_{H}|\gamma^{\star}e^{-}\rangle$$

= $(2\pi)^{4}\delta^{4}(q+p_{1}-p_{2})\bar{u}(p_{2})\gamma^{\mu}u(p_{1})$
× $(-ie)\left[1+\frac{\alpha}{4\pi}\left(-\ln^{2}\frac{\mu^{2}}{Q^{2}}-3\ln\frac{\mu^{2}}{Q^{2}}-8+\frac{\pi^{2}}{6}\right)\right].$ (12)

To confirm that the IR divergences cancel in S_H , without invoking scaleless-integral magic, we can impose physical cutoffs on the degrees of freedom that interact in H_{sc} , such as including only photons with energy less than δ or within angle *R* of an electron [36]. Then the diagrams like \mathcal{M}_B are no longer scaleless. We have checked that all of the IR divergences cancel in S_H using this approach. Although S_H comes out IR finite, it retains sensitivity to the scales *R* and δ ; in pure dimensional regularization, these cutoff scales are replaced by the single scale μ .

With a new definition of the *S* matrix, it is natural to ask, what are its predictions for observables? Consider an infrared-finite observable, such as the total cross section in $Z \rightarrow$ hadrons. To compute it, note that the total cross section for $Z \rightarrow anything$, at order α_s is zero, since the forward scattering $Z \rightarrow Z$ cross section exactly cancels the cross section to everything else. This follows from unitarity, whether using S_H or *S*. Now, the *Z* has no soft or collinear interactions, so $|Z^d\rangle = |Z\rangle$. Thus, $\langle Z|S_H|Z\rangle = \langle Z|S|Z\rangle$ to all orders in perturbation theory. Therefore, the $Z \rightarrow Z$ forward-scattering cross section is the same with S_H and *S* and so is the $Z \rightarrow$ hadrons cross section.

More generally, if we consider an observable less inclusive than the total cross section, such as a jet rate, then the details of the asymptotic dynamics will be important to determining the differential cross section. When we include this dynamics by evolving the final state with an $e^{-iH_{as}t_{+}}$ factor, we would effectively be computing $\sum_{X} |\langle X|e^{-iH_{as}t}S_{H}|Z\rangle|^{2} = \sum_{X} |\langle X|S|Z\rangle|^{2}$, so the differential cross section will agree exactly with one computed using S. Since infrared-safe cross sections computed using S are incontrovertible agreement with data, this is reassuring: we have not created more problems than we have solved with a finite S matrix. On the other hand, there are also issues where physical predictions using Sare ambiguous, such as with charged particles in the initial states. S_H could possibly shed light on these processes.

Having a finite *S* matrix is perhaps most appealing in situations where the *S* matrix is of interest for its own sake, for example, for its mathematical properties. One popular playground for studying the mathematics of the *S* matrix is $\mathcal{N} = 4$ super-Yang-Mills theory. This theory is a conformal gauge field theory. Although its *S* matrix is UV finite, it is still IR divergent. Moreover, its mathematical properties depend on how these IR divergences are removed. For example, the simplest approach is simply to drop the $\frac{1}{c_{IR}}$ terms, $\overline{\text{MS}}$ -style. Doing so for the planar two-loop six-particle amplitude, for example, gives a complicated

function of the nine kinematical invariants. If instead, one employs the Bern-Dixon-Smirnov (BDS)-Ansatz, taking the ratio of the S-matrix element to the exponentiation of the one-loop result [37,38], then the result is a relatively simple "remainder function" of only the three dualconformally invariant cross-ratios [39,40]. While dualconformal invariance is preserved by the BDS-Ansatz, the BDS remainder functions have unappealing analytic properties, such as violating the Steinmann relations [41]. A BDS-like Ansatz might preserve these [42]. A minimal normalization is another option [43]. In the computation of S_H , the IR divergences cancel automatically: The analog of the BDS subtraction comes naturally from multiplying $1/\epsilon$ counterterms for S_H with the finite $\mathcal{O}(\epsilon)$ parts S_H -matrix elements. Thus, S_H -matrix elements provide some of the benefits of IR-finite remainder functions, without the arbitrariness of a ratio. Moreover, as the S_H operator is unitary, properties that follow from unitarity (perhaps including the Steinmann relations) should be automatically satisfied. This is in contrast to remainder functions, which are quotients of S-matrix elements to other quantities.

In this paper, we have argued that there is nothing sacred about the traditional *S* matrix. Its nonperturbative definition is absurdly complicated, and its interaction-picture definition involves an admixture of free and full-theory time evolution. In a theory with massless particles, it is natural to replace the free evolution with universal soft and collinear evolution. Unlike S, whose matrix elements are either infinite (IR divergent) or zero (after exponentiation of the IR divergences), matrix elements of this new object S_H are IR finite to all orders.

In summary, this paper provides the first explicit construction of a *S* matrix for non-Abelian gauge theories with no collinear or soft divergences; it provides rules (see also [44]) for computing S_H beyond just the cancellation of the singularities, allowing the mathematical properties of the *S* matrix to be explored with the IR-divergence problem removed in a natural way; it connects to previous literature on dressed and coherent states but also argues that such nonnormalizable states are not needed for S_H or to compute observables; finally, it connects S_H -matrix elements to SCET and to remainder functions in $\mathcal{N} = 4$ SYM theory for the first time. While there is much still to be understood about S_H , it provides a solid starting point for an improved understanding of scattering in theories with massless particles.

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