



Article Singularities of Scattering Matrices

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Abstract: Our main result is the analysis of singularities of the integrands of integrals representing the matrix elements of the scattering matrix and the inclusive scattering matrix in perturbation theory. These results are proven for any quantum field theory in any dimension.

Keywords: singularity; inclusive scattering matrix; on-shell diagram

1. Introduction

The primary goal of the present paper was the analysis of the inclusive scattering matrix. This analysis led to some results also for the conventional scattering matrix. Namely, in both cases, we obtained some information about the singularities of integrands of corresponding integrals (under certain assumptions). We propose a procedure that allows us to analyze the singularities of integrands for the inclusive scattering matrix by induction. This procedure gives information about the conventional scattering matrix, but it cannot be formulated without using the inclusive scattering matrix.

It was proven in [1] and other papers that the scattering amplitudes for the N = 4 super Yang–Mills theory and those in some other theories can be expressed in terms of on-shell diagrams. We found that, in these cases, the inclusive scattering matrix can also be expressed this way.

Many recent papers have been based on the idea that it is possible to formulate quantum field theory "on-shell" (in terms of particles instead of fields). This idea led to very interesting (but still incomplete) results for four-dimensional massless theories. Our results can be applied in any dimension to any theory. They are incomplete; however, they strongly support this idea.

Our main tools are generalized Green functions (GGreen functions). These functions appear naturally in the formalism of *L*-functionals and in Keldysh formalism. (See [2] for a review of the formalism of *L*-functionals, suggested in [3], and [4–6] for the review of Keldysh formalism).

One can define the inclusive *S*-matrix as an on-shell GGreen function. In the case where the theory has particle interpretation, inclusive cross-sections can be expressed linearly in terms of matrix entries of the inclusive *S*-matrix [2,7,8].

Notice that it is possible to modify our considerations in a way that allows us to analyze the inclusive scattering matrix of quasiparticles (elementary excitations of equilibrium states or, more generally, translation-invariant stationary state).

2. GGreen Functions

One can define generalized Green functions (GGreen functions) in the state ω using the following formula, where *B* is an observable:

 $M = T^{opp}(B^*(\mathbf{x}_{i_1}, t_{i_1}) \dots B^*(\mathbf{x}_{i_s}, t_{i_s}))$

$$G_n^S = \omega(MN) \tag{1}$$

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where

stands for an antichronological product (times increasing) and

$$N = T(B(\mathbf{x}_{j_1}, t_{j_1}) \dots B(\mathbf{x}_{j_{n-s}}, t_{j_{n-s}}))$$

stands for a chronological product (times decreasing). (We consider a state as a positive linear functional on the algebra of observables A. In what follows, we are interested in the case where ω is a ground state; then, $\omega(A)$ denotes the vacuum expectation value (vev). Translations act as automorphisms of A; a spatial translation by \mathbf{x} and a time translation by t transform B into $B(\mathbf{x}, t)$).

The GGreen function depends on the choice of subset *S* of the set $\{1, \dots, n\}$, j_k belongs to *S*, and i_l belongs to the complement of *S*. If *S* coincides with $\{1, \dots, n\}$, the GGreen function is denoted by G_n^+ ; it coincides with the conventional Green function. If *S* is empty, the GGreen function is denoted by G_n^- ; it is a complex conjugate to G_n^+ .

The observable *B* can depend on a discrete variable (spin, polarization, etc.); then, the GGreen function also depends on discrete variables.

Instead of the notation G_n^S , we use the notation $G_n(\mathbf{x}_1, t_1, \epsilon_1, ..., \mathbf{x}_n, t_n, \epsilon_n)$, where $\epsilon_i = \pm 1$. The set *S* is identified with the set of all *i*s obeying $\epsilon_i = +1$. In other words, we take $\epsilon_i = -1$ for operators entering *M* and $\epsilon_i = +1$ for operators entering *N*.

As usual, after Fourier transform, we obtain the GGreen functions in (\mathbf{p}, t) - and (\mathbf{p}, ω) -representations. Notice that in the (\mathbf{p}, ω) representation, the complex conjugate of $G_n(\mathbf{p}_1, \omega_1, \epsilon_1, \ldots, \mathbf{p}_n, \omega_n, \epsilon_n)$ is equal to $G_n(-\mathbf{p}_1, -\omega_1, -\epsilon_1, \ldots, -\mathbf{p}_n, -\omega_n, -\epsilon_n)$ (to $G_n(-\mathbf{p}_1^*, -\omega_1^*, -\epsilon_1, \ldots, -\mathbf{p}_n^*, -\omega_n^*, -\epsilon_n)$ if we consider the analytic extension to complex arguments).

The inclusive cross-section can be expressed in terms of amputated on-shell GGreen functions in (\mathbf{p}, ω) -representation. To obtain this cross-section, we exclude the δ -function corresponding to energy–momentum conservation from the GGreen function; in the remaining expression, we take + variables equal to –variables. More precisely, if we are interested in the collision of two particles with momenta q_1 , q_2 , producing particles with momenta p_1, \ldots, p_n plus some unspecified particles, we should consider amputated GGreen function G_{2n+4} depending on n + 2 on-shell variables $p_1, \ldots, p_n, q_1, q_2$ with $\epsilon = +1$ and n + 2 on-shell variables $p'_1, \ldots, p'_n, q'_1, q'_2$ with $\epsilon = -1$. We should exclude the δ -function from G_{2n+4} and take $p'_i \rightarrow p_i, q'_i \rightarrow q_j$.

We are mostly interested in connected amputated on-shell GGreen functions in (\mathbf{p}, ω) representation. We denote these functions by $\hat{G}_n(p_1, \epsilon_1, \ldots, p_n, \epsilon_n)$. (For simplicity, we
assume that there exists only one type of particle with dispersion law $\omega(\mathbf{p})$; to obtain the
on-shell GGreen function, we take $\omega_i = \omega(\mathbf{p}_i)$ in the amputated GGreen function).

One can prove (see, for example [9]) that the sum of all functions \hat{G}_n vanishes:

$$\sum_{\varepsilon_i=\pm 1} \hat{G}_n(p_1, \epsilon_1, \dots, p_n, \epsilon_n) = 0$$
⁽²⁾

This relation allows us to express the function $\hat{G}_n^+ + \hat{G}_n^-$ in terms of other on-shell GGreen functions.

The relation (2) is closely related to the unitarity of the scattering matrix and to Cutkosky's cutting rules.

In the formalism of *L*-functionals, we work with linear functionals on Weyl algebra (an associative algebra with involution with generators obeying canonical commutation relations). Such a functional (denoted by L_K) corresponds to every trace class operator *K* in all representations of CCR: if *A* is an element of Weyl algebra, then $L_K(A) = TrAK$. A field ϕ generates two operators on the space \mathcal{L} of linear functionals on Weyl algebra; one of them (denoted by ϕ_+) corresponds to the multiplication of *K* by ϕ from the left; the second one (denoted by ϕ_-) corresponds to the multiplication of *K* by ϕ^* from the right. If *K* is a density matrix, L_K is a physical *L*-functional describing a state of our system.

Applying a chronological product of operators $\phi_+(\mathbf{x}_j, t_j)$ and operators $\phi_-(\mathbf{x}_i, t_i)$ to the state ω , we obtain a linear functional on the Weyl algebra. It is easy to check

that by calculating the value of this functional on the unit element of Weyl algebra, we obtain the GGreen function. This remark allows us to construct in the standard way the diagram techniques for the calculation of GGreen functions. The same techniques appear in Keldysh formalism.

The diagram techniques that allow us to calculate GGreen functions in the framework of perturbation theory are very similar to the techniques for conventional Green functions. We need very limited information about the diagrams to calculate GGreen functions. First of all, if we had *n* fields in the original Lagrangian or Hamiltonian, then in the diagrams for GGreen functions, we should have 2n fields (+ and - fields) These diagrams have two types of vertices (+ and - vertices). The crucial property of propagators: the propagators connecting vertices of different types (+- propagators and -+ propagators) are on-shell.

For example, for a relativistic scalar field

$$G_{+-}(p) = \hbar 2\pi \theta(-\omega)\delta(p^2 - m^2), G_{-+}(p) = \hbar 2\pi \theta(\omega)\delta(p^2 - m^2),$$
$$G_{++}(p) = \hbar \frac{i}{p^2 - m^2 + i0}, G_{--} = \hbar \frac{-i}{p^2 - m^2 - i0},$$

where $p = (\omega, \mathbf{p})$ denotes the energy–momentum vector. The vertices contain a factor \hbar^{-1} . (We assume here that the GGreen functions correspond to the ground state, although

our considerations can be applied in more general situations). In what follows, we use the renormalized diagram technique, where the propagators contain the physical dispersion law and are properly normalized. For a relativistic scalar field, this means that *m* is the physical mass.

Our considerations do not depend on Lorentz invariance and locality; therefore, we do not care about divergences.

3. Semiclassical Approximation

Notice that one can obtain a slightly different diagram technique by taking different bases in the space of fields (Keldysh basis or, in a different terminology, physical basis); this technique was used in quantum field theory in [10]. In this basis, we replace ϕ_+ , ϕ_- with

$$\phi^r = rac{1}{2}(\phi_+ + \phi_-), \phi^a = \hbar^{-1}(\phi_+ - \phi_-).$$

(Alternative notations are $\phi^r = \phi_{cl}$ and $\phi^a = \phi_{qu}$, where *cl* stands for classical and *qu* stands for quantum). One can define GGreen functions in terms of these fields; in coordinate representations, they depend on variables $(\mathbf{x}_1, t_1, \sigma_1, \dots, \mathbf{x}_n, t_n, \sigma_n)$, where $\sigma_i = r$ or $\sigma_i = a$. These functions are linear combinations of functions $G_n(\mathbf{x}_1, t_1, \epsilon_1, \dots, \mathbf{x}_n, t_n, \epsilon_n)$ with constant coefficients. The function with all $\sigma_i = a$ is equal to zero; this statement is equivalent to (2). As usual, we can define GGreen functions in \mathbf{p}, t and in \mathbf{p}, ε representations. The inclusive scattering matrix can be expressed in terms of GGreen function $G_n(p_1, \sigma_1, \dots, p_n, \sigma_n) = G_n(\mathbf{p}_1, \varepsilon_1, \sigma_1, \dots, \mathbf{p}_n, \varepsilon_n, \sigma_n)$ on-shell. The diagram technique in the Keldysh basis is very similar to the technique described in Section 2. The propagator can be regarded as a 2 × 2 matrix, where the diagonal entry G_{aa} vanishes and the diagonal entry G_{rr} is on-shell.

For the scalar field, the propagators in the Keldysh basis are

$$G^{rr} = \hbar\pi\delta(p^2 - m^2), G^{aa} = 0, G^{ra} = G^{ar} = \frac{1}{p^2 - m^2 + i\omega 0}$$

It is easy to check that the vertices with indices $rr \dots r$ vanish. A vertex having k indices of type a contains a factor \hbar^{k-1} . It follows that the representation of the inclusive scattering matrix by diagrams in the Keldysh basis contains only non-negative powers of \hbar ; hence, it gives a decomposition of this matrix in Taylor series with respect to \hbar . In particular, the limit of the inclusive scattering matrix as $\hbar \rightarrow 0$ is represented as a sum

of diagrams where all propagators are of the form G^{ra} , G^{ar} and all vertices have only one index of type *a*.

4. On-Shell Diagrams

In on-shell diagrams, edges are oriented; as usual, every edge should carry momentum and every vertex should contain a delta function expressing the conservation of momentum. The propagators should be on-shell (they should have the form $M(p)\delta(\omega - \omega(\mathbf{p}))$ or $M(p)\delta(\omega + \omega(\mathbf{p}))$) and the momenta of all external vertices should be on-shell.

All on-shell diagrams we consider have two types of vertices (+ and - vertices).

It is obvious that any *on-shell GGreen function can be represented as a sum of on-shell diagrams with propagators* $G_{+-}(p)$, $G_{-+}(p)$ and with \hat{G}_n^+ , \hat{G}_n^- as vertices. (Replacing vertices \hat{G}_n^+ and \hat{G}_n^- with diagrams representing these functions, we obtain diagrams for an on-shell GGreen function).

This statement allows us to express all loop level l on-shell GGreen functions in terms of functions \hat{G}_n^+ and \hat{G}_n^- at the loop levels $\leq l$. If the conventional on-shell Green functions \hat{G}_n^+ can be expressed in terms of on-shell data, the same is true for on-shell GGreen functions. In particular, if on-shell Green functions are represented by on-shell diagrams, on-shell GGreen functions are also represented by on-shell diagrams.

BCFW recursion [11] allows us to express scattering amplitudes in terms of simpler scattering amplitudes (at least in the case of vanishing boundary contribution). Combining this fact with the above statements, we obtain that, for all theories, we can express tree-level on-shell GGreen functions in terms of on-shell data (and in the case of gauge theories in terms of on-shell diagrams).

For the N = 4 SUSY Yang–Mills theory, one can express all on-shell Green functions, hence all on-shell GGreen functions in terms of on-shell diagrams.

5. Partial Summation

Lemma 1. The sum of all diagrams for GGreen function $\hat{G}_n(p_1, \epsilon_1, ..., p_n, \epsilon_n)$ containing a + + edge separating $p_1, ..., p_k$ from $p_{k+1}, ..., p_n$ is equal to

$$\int dq G_{++}(q) \hat{G}_k(p_1,\epsilon_1,\ldots,p_k,\epsilon_k,q,+1) \hat{G}_{n-k}(p_{k+1},\epsilon_{k+1},\ldots,p_n,\epsilon_n,-q,+1)$$

The lemma is an obvious generalization of the well-known statement for conventional Green functions.

Let us consider a diagram for a connected on-shell GGreen function with *n* external vertices. Let us remove the edge corresponding to a +- propagator. Denote the remaining part by *A*, we add to this part two external vertices (+ vertex and – vertex) with momenta q, -q where q is an on-shell momentum of the removed edge. The contribution of *A* to the GGreen function will be denoted by $A_{n+2}(p_1, \ldots, p_n, q, -q)$. It is easy to prove the following:

Lemma 2. We can obtain the contribution of the original diagram to the GGreen function by multiplying A_{n+2} by $G_{+-}(q)$ and integrating over q.

Set *A* can be connected or disconnected (the removed +– edge can be non-separating or separating).

Lemma 3. The sum of all diagrams for the on-shell GGreen function $\hat{G}_n(p_1, \epsilon_1, ..., p_n, \epsilon_n)$ containing a + - edge separating $p_1, ..., p_k$ from $p_{k+1}, ..., p_n$ is equal to

$$\int dq G_{+-}(q) \hat{G}_{k+1}(p_1,\epsilon_1,\ldots,p_k,\epsilon_k,q,+1) \hat{G}_{n-k+1}(p_{k+1},\epsilon_{k+1},\ldots,p_n,\epsilon_n,-q,-1)$$

This lemma is similar to Lemma 1; the proof is the same.

Lemma 4. The sum of all diagrams for the on-shell GGreen function $\hat{G}_n(p_1, \epsilon_1, ..., p_n, \epsilon_n)$ containing a non-separating +- edge is equal to

$$\int dq G_{+-}(q) \hat{G}_{n+2}(p_1,\epsilon_1,\ldots,p_n,\epsilon_n,q,+1,-q,-1)$$

To prove Lemma 4, we start with a diagram for the function $\hat{G}_{n+2}(p_1, \epsilon_1, ..., p_n, \epsilon_n, q, +1, q, -1)$. Connecting the vertices with momenta q, -q with a + - edge obtains a diagram for $\hat{G}_n(p_1, \epsilon_1, ..., p_n, \epsilon_n)$ with a non-separating edge. (Recall that all diagrams for the function \hat{G} are connected). All diagrams with a non-separating +- edge can be obtained this way. Now, we can apply Lemma 2.

6. Singularities

The statements in the preceding section can be used to obtain information about singularities of the (inclusive) scattering matrix. In many cases, it is useful to work with integrands of integrals expressing the (inclusive) scattering matrix (see [1,12], etc). It was shown in these papers that, in the case of planar N4 SUSY Yang–Mills, the singularities of these integrands can be used to calculate the integrands. (If we know the singularities of the integrand, we can calculate the integrand up to a regular summand. However, in the situation for planar N = 4 SUSY Yang–Mills, one can also find the complete answer; see [1]). Later, this statement was generalized.

We assume that the singularities (or at least leading singularities) of partial sums are also singularities of the GGreen functions we are studying. Moreover, we assume that a similar statement is true for corresponding integrands. Of course, these statements are not necessarily correct; the singularities of partial sums can cancel the singularities of the remaining summands. (We can apply these statements to any type of singularity, but for the integrands, we are interested in the poles and residues in the poles).

We represent a GGreen function as a sum of Feynman diagrams. A Feynman diagram in every order of perturbation theory is an integral over internal momenta; we represent the GGreen function in a given order of perturbation theory as an integral of the sum of the integrands of individual diagrams. In what follows, talking about the GGreen function, we have in mind the connected GGreen function in a fixed order of perturbation theory. The integrand of an integral representing the GGreen function is not well defined; for example, in gauge theories, it depends on the choice of gauge condition. Talking about an integrand, we have in mind one of these integrands. One can hope that our statements are true for all (or almost all) integrands.

We denote the integrand of GGreen function \hat{G} by \hat{g} . Considering the *l*-loop contribution, we are using the notation \hat{G}^l for the GGreen function and \hat{g}^l for the integrand. The integrand can be considered as a differential form on the space of internal momenta. (Sometimes, it is convenient to consider it as a differential form on the space of internal and external momenta). Notice that the momenta are not independent (or, equivalently, the coefficients of the differential form contain delta functions coming from conservation laws).

In the conditions of Lemma 3, the expression

$$\int dq G_{+-}(q) \sum_{l_1+l_2=l} \hat{g}_k^{l_1}(p_1, \epsilon_1, \dots, p_k, \epsilon_k, q, +1) \hat{g}_{n-k}^{l_2}(p_{k+1}, \epsilon_{k+1}, \dots, p_n, \epsilon_n, -q, -1)$$
(3)

is a partial integrand for on-shell GGreen function $\hat{G}_n^l(p_1, \epsilon_1, \dots, p_n, \epsilon_n)$. It follows from Lemma 4 that

$$\int dq G_{+-}(q) \hat{g}_{n+2}^{l-1}(p_1, \epsilon_1, \dots, p_n, \epsilon_n, q, +1, -q, -1)$$
(4)

is a partial integrand for the same GGreen function.

One can use these statements to describe an inductive procedure that allows us to calculate the singularities of $\hat{g}_n(p_1, \epsilon_1, ..., p_n, \epsilon_n)$. This procedure is similar to the procedure described in [1,12] (see the formula (2.25) in [1]).

The Formulas (3) and (4) do not describe singularities of integrands \hat{g}_n^+ of conventional Green functions \hat{G}_n^+ . Some information about these singularities can be obtained from Lemma 1. We can use (2) to obtain additional information.

Using (2), we derive from Lemma 4 or from the relation (4) that

Lemma 5. $-\int dq G_{+-}(q) \sum' \hat{g}_{n+2}(p_1, \epsilon_1, \dots, p_n, \epsilon_n, q, +1, -q, -1)$ is a partial integrand for the expression $T_n(p_1, \dots, p_n) = (\hat{G}_n^+ + \hat{G}_n^-)(p_1, \dots, p_n)$. (The sign \sum' denotes summation over all $\epsilon_i = \pm 1$ except $\epsilon_1 = \ldots = \epsilon_n = 1$ and $\epsilon_1 = \ldots = \epsilon_n = -1$.)

This statement allows us to obtain information about the singularities of the integrand of T_n and therefore about the singularities of the integrands of \hat{G}_n^+ and \hat{G}_n^- .

Additional information about singularities of T_n can be obtained in the same way from (2) and (3).

Lemma 6. $-\sum' \int dq G_{+-}(q) \sum_{l_1+l_2=l} \hat{g}_k^{l_1}(p_1, \epsilon_1, \dots, p_k, \epsilon_k, q, +1) \hat{g}_{n-k}^{l_2}(p_{k+1}, \epsilon_{k+1}, \dots, p_n, \epsilon_n, -q, -1)$ is a partial integrand for the expression $T_n(p_1, \dots, p_n) = (\hat{G}_n^+ + \hat{G}_n^-)(p_1, \dots, p_n)$. (The sign Σ' denotes summation over all $\epsilon_i = \pm 1$ except $\epsilon_1 = \ldots = \epsilon_n = 1$ and $\epsilon_1 = \ldots = \epsilon_n = -1$.)

Now, we can suggest an inductive procedure that allows us to obtain information about the singularities of integrands for on-shell GGreen functions. Calculating \hat{g}_n , we denote by $\hat{g}_n^{l,s}$ the contribution of the diagrams with the number of loops $\leq l$ and the number of +- and -+ propagators $\leq s$. Using Lemma 5, we obtain information about the singularities of $\hat{g}_n^{l,s}$ from the information about the singularities of $\hat{g}_{n+2}^{l-1,s-1}$. Using (3), we obtain information about the singularities of $\hat{g}_n^{l,s-1}$. As a result, we obtain information about the singularities of $\hat{g}_n^{l,s}$ from the information about the singularities of $\hat{g}_n^{l,s-1}$. As a result, we obtain information about the singularities of $\hat{g}_n^{l,s}$ from the information about the singularities of $\hat{g}_n^{l,s}$.

To calculate singularities of $\hat{g}_n^{l,0}$, we should know the singularities of the *l*-loop contribution to \hat{g}_k for $k \leq n$. The information about these singularities can be obtained from Lemmas 1 and 5 if we know the singularities of $\hat{g}_k^{l-1,s}$.

In Lorentz-invariant theories, the integrands are rational functions. (We consider $\delta(x)$ as a rational function of x because it can be expressed as a linear combination of two fractions $\frac{1}{x\pm i0}$.) Therefore, one can hope that the above statements describe all singularities. (In other theories, additional singularities come from the singularities of the dispersion law).

7. Relation to Positive Grassmannian

It seems that deep relations with cluster algebras and a positive Grassmannian discovered in [1] for the N=4 SUSY Yang–Mills are very general. They are based first of all on the consideration of on-shell diagrams with two types of vertices (bicolored graphs in mathematical terminology). Such diagrams also appear in our approach (however, the origin of the two types of vertices is completely different). To relate these diagrams to a positive Grassmannian and cluster algebras, one notices that a planar diagram of this kind (planar bicolored graph = plabic graph) specifies a positroid (a cell in a cell decomposition of a positive Grassmannian) and a cluster in the corresponding cluster algebra. Different plabic graphs specify the same positroid if they are related based on a sequence of local moves (cluster transformations in the language of cluster algebras). The relation to physics was derived in [1] from the remark that these moves do not change the amplitude corresponding to an on-shell diagram. If this remark could be generalized to our situation, we would be able to use the techniques of the positive Grassmannian.

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