

GENERAL SUBTRACTION METHOD FOR NUMERICAL CALCULATION OF ONE-LOOP QCD MATRIX ELEMENTS*

ZOLTÁN NAGY

Institute for Theoretical Physics, University of Zürich
Winterthurerstrasse 190, 8057 Zürich, Switzerland

AND DAVISON E. SOPER

Institute of Theoretical Science, University of Oregon
Eugene, OR 97403-5203, USA

(Received October 11, 2004)

We present a subtraction scheme for eliminating the ultraviolet, soft, and collinear divergences in the numerical calculation of an arbitrary one-loop QCD amplitude with an arbitrary number of external legs. The subtractions consist of local counter terms in the space of the four-dimensional loop momentum.

PACS numbers: 11.15.Bt

1. Introduction

Tests of the Standard Model or one of its extensions frequently involve high momentum transfer processes in which one is looking for effects from new interactions or particles. In most cases, at least some of the particles interact via the strong interactions. Then, in order to obtain reasonably accurate predictions for the expected cross sections, it is necessary to calculate the cross section at next-to-leading order (NLO) in quantum chromodynamics (QCD). Sometimes this is possible using the currently available theoretical tools, sometimes not. This paper concerns a method for potentially extending the range of problems for which a next-to-leading order calculation is possible.

* Presented at the final meeting of the European Network “Physics at Colliders”, Montpellier, France, September 26–27, 2004.

An NLO calculation necessarily involves a virtual loop integration. That is, one has an integral

$$\int \frac{d^d l}{(2\pi)^d} \tilde{\Gamma}(k_1, \dots, k_n; l)$$

over a loop momentum l in $d = 4 - 2\varepsilon$ dimensions, with momenta $k_1, \dots, k_n$ leaving the graph at vertices around the loop. Of course, one wants $d = 4$ in the end, but there can be infrared divergences, which are temporarily regulated by working with $d \neq 4$. (There can also be ultraviolet divergences, but we ignore these for this initial discussion.) The infrared divergences arise because we work with a gauge theory containing massless particles. This leads to poles of the form $1/\varepsilon^2$ and $1/\varepsilon$ in the integral.

The traditional method of dealing with the 1-loop integrals initiated in the context of collider physics cross sections by Ellis, Ross, and Terrano [1], is to calculate the integrals analytically. The result is expressed in the form of the residues of the $1/\varepsilon^2$ and $1/\varepsilon$ poles and a remaining finite piece, which contains the most important physical information. There are several one-loop amplitude have been calculated up to $n = 5$ [1] and there are also calculations available with massive particles, such as massive quarks.

One wonders if we could not get beyond $n = 5$ by simply performing the virtual loop integrals numerically. Of course, one is not going to perform integrals in $d = 4 - 2\varepsilon$ dimensions numerically. Instead, one would have to do something about the infrared divergences first, then take $d = 4$. Something like this was tried in Ref. [2] in the case of $e^+ + e^- \rightarrow 3 \text{ jets}$.

In this paper, we present a different proposal, one that is very close to the traditional method. One would subtract from the integrand certain simple integrands that match the complete integrand in one of the soft or collinear limits that gives a divergence. Then the difference would be integrable in $d = 4$ dimensions and this integral would be performed numerically. The integral of each subtraction term would be added back, but this time with the integration performed analytically. This gives the same $1/\varepsilon^2$ and $1/\varepsilon$ poles that one has in an analytic calculation, ready for cancellation as usual.

There has been other recent work aimed at automating the calculation of loop integrals in such a way that those integrals that are not amenable to analytic evaluation could be evaluated numerically [3]. This approach makes use of the Feynman parameter representation of the diagrams.

This paper provides only a short review of our subtraction method. The details of the scheme can be found in Ref. [4].

2. Matrix elements at one-loop level

2.1. One-loop graphs

As discussed in the introduction of this section, we wish to calculate the one-loop, m -parton matrix element graph by graph using numerical integration. In this subsection, we define some tools for this calculation. We use the vector notation in color and spin space of the previous subsection to write the one-loop matrix element as a sum of the one-loop Feynman graphs,

$$|\mathcal{M}(p_1, \dots, p_m)\rangle = \sum_{\text{graphs } G} |\mathcal{G}(G; p_1, \dots, p_m)\rangle. \quad (1)$$

The $|\mathcal{G}\rangle$ vector is related to the one-loop, amputated Green function.

The graph G contains a one-loop, one-particle-irreducible subgraph Γ with $n = n(G)$ external lines and n internal lines around the loop. Let us label momenta of the internal lines $l_1, l_2, \dots, l_n$. We integrate over the loop momentum. One can consider l_k for some specific index k to be the independent loop momentum, which we call l . In the actual numerical integration, one chooses a definition for l , then chooses a random value for l thus defined, and then computes the l_i . Thus our notation is

$$|\mathcal{G}(G; p_1, \dots, p_m)\rangle = \int \frac{d^d l}{(2\pi)^d} |\tilde{\mathcal{G}}(G; \{l\}; p_1, \dots, p_m)\rangle, \quad (2)$$

where $\tilde{\mathcal{G}}$ denotes the integrand for graph G and $\{l\}$ is a shorthand for $l_1, \dots, l_n$.

In certain graphs, the loop integration could be infrared and/or ultra-violet divergent. To handle the infrared divergences, we introduce simple counter terms that we subtract from the integrand for the numerical integration and then add back analytically. We discuss this in Sections 3, 4, 5.

2.2. S -matrix

The S -matrix can be constructed from the amputated Green functions by means of the LSZ reduction formula

$$|\mathcal{M}_{\text{full}}(p_1, \dots, p_m)\rangle = \left(\prod_i \sqrt{r_i} \right) |\mathcal{M}_{\text{full}}^{(T)}(p_1, \dots, p_m)\rangle. \quad (3)$$

Here we consider both sides of the equation to be vectors in color and spin space. The subscripts “full” indicate that this formula applies to the matrix element summed over orders of perturbation theory. The T (for “truncated”) superscript on $\mathcal{M}$ on the right indicates that the matrix element is calculated

by multiplying amputated Green functions by the appropriate Dirac spinors and polarization vectors. The factors $\sqrt{r_i}$, one for each external particle, are of two types, one for gluons and one for quarks and antiquarks. They are defined from the residues of the poles of the corresponding renormalized propagators at $p^2 = 0$.

The constants r_i have perturbative expansions

$$r_i = 1 + r_i^{(1)} + \cdots, \quad (4)$$

where $r_i^{(1)} \propto \alpha_s^1$. Thus, including terms up to one-loop order,

$$\begin{aligned} |\mathcal{M}_{\text{full}}(p_1, \dots, p_m)\rangle &= |\mathcal{M}_{\text{tree}}(p_1, \dots, p_m)\rangle + |\mathcal{M}^{(T,1)}(p_1, \dots, p_m)\rangle \\ &+ \sum_i \frac{1}{2} r_i^{(1)} |\mathcal{M}_{\text{tree}}(p_1, \dots, p_m)\rangle. \end{aligned} \quad (5)$$

Here $|\mathcal{M}^{(T,1)}\rangle$ is the one-loop contribution to $|\mathcal{M}^{(T)}\rangle$. Elsewhere in this paper we denote $|\mathcal{M}^{(T,1)}\rangle$ simply as $|\mathcal{M}\rangle$.

Now we need to evaluate the residue constants $r_i^{(1)}$ and we can obtain the results from the one-loop expressions of the renormalized propagators. For the quark lines we have

$$r_q^{(1)} = C_F \frac{\alpha_s}{4\pi} \frac{1}{\varepsilon} \frac{(4\pi)^\varepsilon}{\Gamma(1-\varepsilon)} \quad (6)$$

and for the gluons

$$r_g^{(1)} = - \left[\frac{5}{3} C_A - \frac{4}{3} T_R n_f \right] \frac{\alpha_s}{4\pi} \frac{1}{\varepsilon} \frac{(4\pi)^\varepsilon}{\Gamma(1-\varepsilon)}, \quad (7)$$

where $T_R = 1/2$ and n_f is the number of quark flavors.

3. Renormalization

The ultraviolet divergences are to be eliminated according to the $\overline{\text{MS}}$ renormalization prescription. However, since we calculate loop integrals by numerical integration, the implementation of the $\overline{\text{MS}}$ prescription needs some analysis. This is the subject of the present section.

Consider an ultraviolet divergent one-loop graph with n propagators in the loop. Here n could be 2, 3, or 4. Denote the momenta leaving Γ by $k_1, \dots, k_n$. In our application, Γ will be a subgraph of G and the momenta $k_1, \dots, k_n$ will be linear combinations of $p_1, \dots, p_m$. The graph Γ has the generic form

$$\Gamma(k_1, \dots, k_n) = \int \frac{d^d l}{(2\pi)^d} \tilde{\Gamma}(k_1, \dots, k_n; l). \quad (8)$$

The functions Γ and $\tilde{\Gamma}$ may carry spinor and vector indices as well as color indices. Our notation here suppresses these indices. We seek to calculate the renormalized version of Γ . With $\overline{\text{MS}}$ renormalization, this is

$$[\Gamma]_R = \lim_{\varepsilon \rightarrow 0} \left\{ \Gamma - [\Gamma]_{\text{pole}} \right\}, \quad (9)$$

where

$$[\Gamma]_{\text{pole}} = \frac{1}{\varepsilon} \frac{(4\pi)^\varepsilon}{\Gamma(1-\varepsilon)} \times \lim_{\varepsilon \rightarrow 0} [\varepsilon \Gamma(\varepsilon)]. \quad (10)$$

Here we are to choose the external momenta so that Γ does not have infrared divergences. For instance, all of the external momenta can be space-like. Then the only pole present in $\Gamma(\varepsilon)$ in Eq. (10) is the ultraviolet pole that is to be removed by renormalization.

Since we are performing integrals numerically, we need to represent $[\Gamma]_{\text{pole}}$ as an integral

$$[\Gamma]_{\text{pole}} = \int \frac{d^d l}{(2\pi)^d} \tilde{\Gamma}_{\text{UV}}(k_1, \dots, k_n; l), \quad (11)$$

in such a way that $[\Gamma]_R$ can be calculated as

$$[\Gamma]_R = \int \frac{d^d l}{(2\pi)^d} \lim_{\varepsilon \rightarrow 0} \left\{ \tilde{\Gamma}(k_1, \dots, k_n; l) - \tilde{\Gamma}_{\text{UV}}(k_1, \dots, k_n; l) \right\}. \quad (12)$$

This last step is justified if the integrands $\tilde{\Gamma}$ and $\tilde{\Gamma}_{\text{UV}}$ match up to an l^{-5} remainder for $l \rightarrow \infty$ at fixed ε and if $\tilde{\Gamma}_{\text{UV}}$ is free of infrared singularities.

There is more than one possibility for $\tilde{\Gamma}_{\text{UV}}$. However, there is a simple prescription that works in all cases save one, the one-loop gluon self-energy, which has a quadratic divergence and needs a more elaborate treatment.

Having a renormalization counterterm for a divergent subgraph Γ of a graph G the renormalized graph can be written by

$$\int \frac{d^d l}{(2\pi)^d} \left\{ |\tilde{\mathcal{G}}(G; \{l\}; p_1, \dots, p_m)\rangle - |\tilde{\mathcal{R}}(G; \{l\}; p_1, \dots, p_m)\rangle \right\}, \quad (13)$$

where $|\tilde{\mathcal{R}}(G; \{l\}; \{p\}_m)\rangle$ is obtained from G by substituting $\tilde{\Gamma}_{\text{UV}}$ for $\tilde{\Gamma}$. In the case that graph G is ultraviolet finite, we define $|\tilde{\mathcal{R}}(G; \{l\}; p_1, \dots, p_m)\rangle$ to be zero. We will use this notation in subsequent sections.

4. Soft singularities

The integrand of a one-loop graph becomes singular when the momentum of an internal gluon loop line that connects to two external lines becomes soft. Consider a one-loop graph G with external momenta $p_1, \dots, p_m$ directed out of the graph. Choose two of the external lines, with labels i and j . If the lines i and j connect via three-point vertices to the two ends of a gluon propagator in the loop, then we will say that $\{i, j\}$ is in the soft indices class for graph G , $\{i, j\} \in I_S(G)$. In this case the integrand $|\tilde{\mathcal{G}}(G; \{l\}; p_1, \dots, p_m)\rangle$ is singular in the limit that the momentum of the gluon propagator that connects lines i and j , call it l_k , tends to zero. The loop integration is logarithmically divergent at this point.

The denominators that become singular in the soft limit $l_k \rightarrow 0$ are l_k^2 for the soft gluon propagator, $(l_k + p_i)^2$ for the immediately preceding propagator in the loop and $(l_k - p_j)^2$ for the immediately following propagator¹. It is useful to define a soft limit function

$$|f_{ij}^S(G; \{p\}_m)\rangle = \lim_{l_k \rightarrow 0} l_k^2 (l_k + p_i)^2 (l_k - p_j)^2 |\tilde{\mathcal{G}}(G; l_1, \dots, l_n; \{p\}_m)\rangle. \quad (14)$$

With this definition, $|f_{ij}^S\rangle$ vanishes if $\{i, j\} \notin I_S(G)$. We can then define a soft subtraction for the integrand $\tilde{\mathcal{G}}$ as

$$|\tilde{\mathcal{S}}_{ij}(G; l_k; \{p\}_m)\rangle = \frac{|f_{ij}^S(G; \{p\}_m)\rangle}{(l_k^2 + i0)((l_k + p_i)^2 + i0)((l_k - p_j)^2 + i0)}. \quad (15)$$

The integral for the original graph minus this subtraction is

$$\int \frac{d^d l}{(2\pi)^d} \left\{ |\tilde{\mathcal{G}}(G; \{l\}; \{p\}_m)\rangle - |\tilde{\mathcal{S}}_{ij}(G; l_k; \{p\}_m)\rangle \right\}. \quad (16)$$

Having subtracted the integral of $|\tilde{\mathcal{S}}_{ij}\rangle$, we should add it back. For this purpose, we need to study the structure of the soft subtraction in more detail. The soft limit function has a rather simple form

$$|f_{ij}^S(G; \{p\}_m)\rangle = -ig_s^2 \mu^{2\varepsilon} 4p_i \cdot p_j \mathbf{T}_i \cdot \mathbf{T}_j \mathbf{H}_{ij} |\mathcal{G}(G_{ij}(G); \{p\}_m)\rangle, \quad (17)$$

where the graph $G_{ij}(G)$ represents the tree level amputated graph obtained from graph G by omitting the three singular propagators and the vertices where they join the external lines i and j . The operator $\mathbf{T}_i \cdot \mathbf{T}_j$ acts in the color space of the i, j external lines and it represents the color connection between them. The $\mathbf{H}_{ij}$ is an operator in the spin space of the partons i and

¹ Here we choose the positive direction around the loop to be from line i to line j .

j and does not depend on the loop momentum. The form of $\mathbf{H}_{ij}$ depends on whether partons i and j are quarks (or equivalently antiquarks) or gluons.

With this result, the soft subtraction is

$$|\tilde{\mathcal{S}}_{ij}(G; l_k; \{p\}_m)\rangle = E_{ij}(l_k, p_i, p_j) \mathbf{T}_i \cdot \mathbf{T}_j \mathbf{H}_{ij} |\mathcal{G}(G_{ij}(G); \{p\}_m)\rangle, \quad (18)$$

where the $E_{ij}(l_k, p_i, p_j)$ is the familiar eikonal factor [5],

$$E_{ij}(l_k, p_i, p_j) = -ig_s^2 \mu^{2\epsilon} \frac{4p_i \cdot p_j}{(l_k^2 + i0)((l_k + p_i)^2 + i0)((l_k - p_j)^2 + i0)}. \quad (19)$$

We need to add back the sum over graphs of the integral $|\mathcal{S}_{ij}\rangle$ of $|\tilde{\mathcal{S}}_{ij}\rangle$. We are now prepared to calculate what this quantity is. Defining $\mathcal{V}_{ij}^{\text{soft}}(\epsilon)$ to be the integral of $E_{ij}(l)$, we have

$$|\mathcal{S}_{ij}(G; \{p\}_m)\rangle = \mathcal{V}_{ij}^{\text{soft}}(\epsilon) \mathbf{T}_i \cdot \mathbf{T}_j \mathbf{H}_{ij} |\tilde{\mathcal{G}}(G_{ij}(G); \{p\}_m)\rangle. \quad (20)$$

The integral can be performed analytically, with the result

$$\mathcal{V}_{ij}^{\text{soft}}(\epsilon) \equiv \int \frac{d^d l}{(2\pi)^d} E_{ij}(l) = \frac{\alpha_s}{4\pi} \frac{(4\pi)^\epsilon}{\Gamma(1-\epsilon)} \left(\frac{\mu^2}{-2p_i \cdot p_j} \right)^\epsilon \left(\frac{2}{\epsilon^2} + \mathcal{O}(\epsilon) \right). \quad (21)$$

Thus $|\mathcal{S}_{ij}(G)\rangle$ is a known integral times a tree level graph with a modified color factor and a kinematic factor $\mathbf{H}_{ij}$.

The sum over graphs G of the subtraction terms is even simpler. We consider a given set of final state parton flavors and a given choice of $\{i, j\}$. The tree graphs $G_{ij}(G)$ have the same parton flavors and momenta. Summing over all graphs G for which $\{i, j\} \in I_S(G)$, the graphs $G_{ij}(G)$ cover all tree graphs with this choice of external partons. Thus summing over graphs G gives the full tree amplitude $|\mathcal{M}_{\text{tree}}(p_1, \dots, p_m)\rangle$ corresponding to the given final state. On the other hand the tree level matrix element is gauge invariant and it ensures that the complicated terms in the operator $\mathbf{H}_{ij}$, do not contribute, so that $\mathbf{H}_{ij}$ can be replaced by the unit operator. Then the soft contribution that we need to add back is

$$\sum_G |\mathcal{S}_{ij}(G; p_1, \dots, p_m)\rangle = \mathcal{V}_{ij}^{\text{soft}}(\epsilon) \mathbf{T}_i \cdot \mathbf{T}_j |\mathcal{M}_{\text{tree}}(p_1, \dots, p_m)\rangle. \quad (22)$$

We now summarize the soft gluon subtractions, this time including a sum over pairs of indices $\{i, j\}$. We subtract

$$\sum_{\{i, j\} \in I_S(G)} |\tilde{\mathcal{S}}_{ij}(G; l_k; p_1, \dots, p_m)\rangle, \quad (23)$$

defined in Eq. (15) from the integrand $|\tilde{\mathcal{G}}(G; \{l\}, p_1, \dots, p_m)\rangle$ for each one-loop graph G . Then we add the integrals of these terms back in the form

$$\sum_{\{i,j\}} \mathcal{V}_{ij}^{\text{soft}}(\varepsilon) \mathbf{T}_i \cdot \mathbf{T}_j |\mathcal{M}_{\text{tree}}(p_1, \dots, p_m)\rangle. \quad (24)$$

5. Collinear singularities

One-loop graphs have logarithmic infrared divergences that arise from integration regions in which the momentum on an internal loop line that connects to an external line becomes collinear with the momentum of the external line. In this section, we define a term that, when subtracted from the graph, eliminates the divergence. This construction is quite similar to what we needed for soft gluon divergences. However, the structure of the collinear subtraction term is more complicated, so we will need a more involved analysis.

Consider a one-loop graph G with external momenta $p_1, p_2, \dots, p_m$ directed out of the graph. Choose one of the external lines, with label i . If the line i connects via a three-point vertex to the loop, and if the loop partons are both gluons or are one gluon and one quark or antiquark, then we will say that i is in the collinear index class for graph G , $i \in I_C(G)$. In this case the loop integration has a logarithmic divergence arising from the region in which the momenta of the loop propagators that connect to line i , call them j and $j+1$, become collinear to the outgoing momentum of line i ,

$$l_j \rightarrow x p_i, \quad -l_{j+1} \rightarrow (1-x) p_i, \quad (25)$$

with $0 < x < 1$.

The denominators that become singular in the collinear limit (25) are l_j^2 and $(-l_{j+1})^2 = (p_i - l_j)^2$. The coefficient of $1/[l_j^2 \times (p_i - l_j)^2]$ in the integrand for the graph is non-singular in the collinear limit. It is useful to define a collinear coefficient function $|f_i^{C,0}(G; x; p_1, \dots, p_m)\rangle$ by

$$|f_i^{C,0}(G; x; \{p\}_m)\rangle = \lim_{l_j \rightarrow x p_i} l_j^2 (p_i - l_j)^2 |\tilde{\mathcal{G}}(G; l_1, \dots, l_n; \{p\}_m)\rangle. \quad (26)$$

One can use the collinear coefficient function to remove the collinear divergence. Consider the integral

$$\begin{aligned} \int \frac{d^d l}{(2\pi)^d} & \left\{ |\tilde{\mathcal{G}}(G; \{l\}, \{p\}_m)\rangle - \frac{1}{(l_j^2 + i0)((p_i - l_j)^2 + i0)} \right. \\ & \times \left. \int dx \delta\left(x - \frac{l_j \cdot n_i}{p_i \cdot n_i}\right) |f_i^{C,0}(G; x; \{p\}_m)\rangle \right\}. \end{aligned} \quad (27)$$

Here we define the momentum fraction x away from the collinear limit by using a lightlike vector n_i . A good choice for n_i is

$$n_i^\mu = -p_i^\mu + \frac{2p_i \cdot w}{w^2} w^\mu, \quad w^\mu = \sum_{k \in \text{final state}} p_k^\mu. \quad (28)$$

By construction, the integral in Eq. (27) does *not* have a divergence from the collinear region (25). The divergence was only logarithmic and the subtraction removes the leading singularity, leaving at worst an integrable singularity.

There are two problems with Eq. (27). The first is that the naive collinear formulae is soft singular if one of the collinear loop lines is a gluon. But all the soft singularities have been subtracted and we do not want to introduce fake soft singularities with the collinear counterterms. In order to cancel these contributions to the net integrand in the collinear limit, we should subtract them from the collinear subtraction term in Eq. (27). To this end, we define a revised collinear coefficient function $|f_i^C(G; x; \{p\}_m)\rangle$

$$\begin{aligned} |f_i^C(G; x; \{p\}_m)\rangle &= |f_i^{C,0}(G; x; \{p\}_m)\rangle - \frac{1}{x} \lim_{y \rightarrow 0} y |f_i^{C,0}(G; y; \{p\}_m)\rangle \\ &\quad - \frac{1}{1-x} \lim_{y \rightarrow 1} (1-y) |f_i^{C,0}(G; y; \{p\}_m)\rangle. \end{aligned} \quad (29)$$

With this coefficient function, our subtraction inside the loop integral is

$$\frac{1}{(l_j^2 + i0)((p_i - l_j)^2 + i0)} \int_0^1 dx \delta\left(x - \frac{l_j \cdot n_i}{p_i \cdot n_i}\right) |f_i^C(G; x; \{p\}_m)\rangle. \quad (30)$$

A second problem remains with Eq. (30). The integral of the subtraction term is ultraviolet divergent. We can easily fix that by modifying the subtraction term to be

$$\frac{f_{\text{UV}}(l_j, l_j - p_i)}{(l_j^2 + i0)((p_i - l_j)^2 + i0)} \int_0^1 dx \delta\left(x - \frac{l_j \cdot n_i}{p_i \cdot n_i}\right) |f_i^C(G; x; p_1, \dots, p_m)\rangle, \quad (31)$$

where

$$f_{\text{UV}}(l_j, l_j - p_i) = \frac{1}{2} \left(\frac{-\mu^2 e}{l_j^2 - \mu^2 e + i0} + \frac{-\mu^2 e}{(l_j - p_i)^2 - \mu^2 e + i0} \right). \quad (32)$$

Here μ is the $\overline{\text{MS}}$ renormalization scale and $e = 2.71828\dots$ is the base of natural logarithms. The factor f_{UV} provides an extra power of l_j^2 in the denominator for large l_j but equals 1 in the collinear limit.

In summary, we subtract from the integrand for each graph G collinear subtraction terms

$$\sum_{i \in I_C(G)} |\tilde{\mathcal{C}}_i(G; \{l\}, p_1, \dots, p_m)\rangle, \quad (33)$$

where

$$\begin{aligned} |\tilde{\mathcal{C}}_i(G; \{l\}, \{p\}_m)\rangle &= \frac{f_{\text{UV}}(l_j, l_j - p_i)}{(l_j^2 + i0)((p_i - l_j)^2 + i0)} \\ &\times \int_0^1 dx \, \delta\left(x - \frac{l_j \cdot n_i}{p_i \cdot n_i}\right) |f_i^C(G; x; \{p\}_m)\rangle. \end{aligned} \quad (34)$$

These subtractions, together with the soft subtractions, remove all of the infrared divergences from the loop integrals.

Our next task, pursued in the following two subsections, will be to add back the subtraction terms $|\tilde{\mathcal{C}}_i(G; \{l\}, p_1, \dots, p_m)\rangle$, this time integrated and summed over graphs G .

5.1. Graph sum of the collinear subtractions

We must add the collinear subtractions $|\mathcal{C}_i(G; p_1, \dots, p_m)\rangle$ back, this time performing the integral analytically. We consider the case that line i is a quark line. The case that i is an antiquark line follows trivially and is covered at the end of this section. The case that i is a gluon line is treated in the very similar way and the result has the same structure as in the quark line case.

We begin by setting up a useful notation. By assumption, line i , carrying momentum p_i out of the graph, connects to a virtual loop in G . Line i must, therefore, connect to the loop at a quark–gluon–quark vertex. We choose to label the propagators in the loop so that the gluon line in the loop has label j and the quark line has label $j + 1$. Thus a gluon line with label j carries momentum l_j into the vertex and the quark line with label $j + 1$ carries momentum $-l_{j+1} = p_i - l_j$ into the vertex. We write the integral for the graph as

$$\begin{aligned} \mathcal{G}(G, p_1, \dots, p_m)^\alpha &= ig_s \mu^\varepsilon T_{\alpha\alpha'}^a \int \frac{d^d l_j}{(2\pi)^d} \frac{1}{(l_j^2 + i0)((p_i - l_j)^2 + i0)} \\ &\times \bar{u}(p_i) \gamma_\mu(p_i - l_j) [\tilde{\mathbf{V}}^\mu(G_i, p_1, \dots, p_i - l_j, \dots, p_m, l_j)]_{\alpha'}^a. \end{aligned} \quad (35)$$

Here we have abandoned our vector notation for spin and color space and written the spin and color indices that are needed for the calculation explicitly. We display a quark color index α for quark line i in $\mathcal{G}$, leaving the other

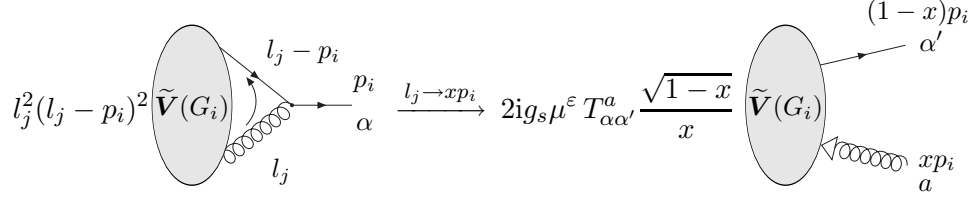


Fig. 1. Illustration of Eq. (36). The left hand side represents $f_i^{C,0}(G; x; \{p\}_m)^\alpha$, which is defined in Eq. (26) as the collinear limit of $l_j^2(l_j - p_i)^2$ times the integrand.

indices on $\mathcal{G}$ unwritten. The amplitude $\tilde{V}$ has a color index a corresponding to the gluon j in the loop and a quark color index α' corresponding to the quark line $j + 1$ in the loop. There is an explicit color matrix $T_{\alpha\alpha'}^a$ connecting the colors of $\tilde{V}$ to the color of $\mathcal{G}$. The amplitude $\tilde{V}$ carries a vector index μ corresponding to the polarization of the gluon line j . It also carries a Dirac spinor index for the quark line $j + 1$. However, we use the matrix notation for the Dirac structure of this line without displaying the Dirac indices explicitly. The Dirac spinor $\bar{u}(p_i)$ represents the final state quark on line i . We have displayed the integration over the loop momentum l_j , the quark–gluon–quark vertex and the propagators for the quark and the gluon in the loop. Everything else is included in the Feynman amplitude $\tilde{V}$ for the amputated tree level graph G_i obtained by omitting the propagators j and $j + 1$ and the vertex that attaches these propagators to external line i in graph G .

With the notation thus defined, we are ready to calculate. The subtraction term $f^{C,0}$ defined in Eq. (26) can be expressed in terms of $\tilde{V}$ as

$$f_i^{C,0}(G; x; p_1, \dots, p_m)^\alpha = 2ig_s\mu^\epsilon T_{\alpha\alpha'}^a \frac{\sqrt{1-x}}{x} (xp_i)_\mu \bar{u}((1-x)p_i) \times [\tilde{V}^\mu(G_i, p_1, \dots, (1-x)p_i, \dots, p_m, xp_i)]_{\alpha'}^a. \quad (36)$$

This equation is illustrated in Fig. 1.

We would now like to sum over graphs. We are considering the collinear subtraction for parton i , which we assume here is a quark and we need consider only graphs that have a collinear divergence for external leg i : $i \in I_C(G)$. Let us call this class of graphs C .

The corresponding graphs G_i are amputated tree graphs with $m + 1$ external legs. The flavors of the first m external particles are $\{f_1, \dots, f_m\}$, the same as for the graph G . The momenta of these particles are the same as for G except for particle i , which carries momentum $(1-x)p_i$ instead of p_i .

The external particle with index $m+1$ is a gluon with momentum xp_i . Let us call the set of all such graphs C' . When we sum over all graphs $G \in C$, the graphs G_i include all graphs in C' except for the graphs in which gluon $m+1$ couples directly to quark i . These graphs are absent because graphs with a self-energy insertion on external line i are *not* included in C . Let us call the set of $(m+1)$ -particle graphs that we do get C'_+ and the graphs that we do not get C'_- .

The collinear subtraction defined in Eq. (34), summed over graphs $G \in C$ is

$$\begin{aligned} \sum_{G \in C} \mathcal{C}_i(G; \{p\}_m)^\alpha &= 2ig_s\mu^\varepsilon T_{\alpha\alpha'}^a \int \frac{d^d l_j}{(2\pi)^d} \frac{f_{UV}(l_j, l_j - p_i)}{(l_j^2 + i0)((p_i - l_j)^2 + i0)} \\ &\times \int \frac{dx}{x} \delta\left(x - \frac{l_j \cdot n_i}{p_i \cdot n_i}\right) \left\{ (1-x) H_{\alpha'}^a(x; \{p\}_m) - H_{\alpha'}^a(0, \{p\}_m) \right\}, \quad (37) \end{aligned}$$

where

$$\begin{aligned} H_{\alpha'}^a(x; p_1, \dots, p_m) &= (1-x)^{-1/2} \\ &\times \lim_{q \rightarrow xp_i} \sum_{G_i \in C'_+} q_\mu \bar{u}((1-x)p_i) [\tilde{\mathbf{V}}^\mu(G_i, p_1, \dots, (1-x)p_i, \dots, p_m, q)]_{\alpha'}^a. \quad (38) \end{aligned}$$

We now note that gauge invariance says something about H . We have inserted a gluon line carrying momentum q almost everywhere into tree graphs with m legs. The gluon has polarization q^μ . Gauge invariance tells us that if we inserted this gluon everywhere, that is if we summed over the entire set of graphs C' , we would get zero. However, we have summed only over the graphs in C'_+ , leaving out the graphs in C'_- . Thus H equals the negative of the sum over graphs in C'_- . This enables us to calculate H as follows

$$\begin{aligned} H_{\alpha'}^a(x; \{p\}_m) &= - \lim_{q \rightarrow xp_i} \sum_{G_i \in C'_-} \frac{q_\mu \bar{u}((1-x)p_i)}{\sqrt{1-x}} \\ &\times [\tilde{\mathbf{V}}^\mu(G_i, p_1, \dots, (1-x)p_i, \dots, p_m, q)]_{\alpha'}^a \\ &= \lim_{q \rightarrow xp_i} \sum_{G'_i \in C_0} (1-x)^{-1/2} g_s\mu^\varepsilon T_{\alpha'\alpha''}^a \\ &\times \frac{\bar{u}((1-x)p_i) \not{q} ((1-x)\not{p}_i + \not{q})}{((1-x)p_i + q)^2 + i0} \\ &\times [\tilde{\mathbf{W}}(G'_i, p_1, \dots, (1-x)p_i + q, \dots, p_m)]_{\alpha''}^a \\ &= g_s\mu^\varepsilon T_{\alpha'\alpha''}^a \mathcal{M}(p_1, \dots, p_i, \dots, p_m)^{\alpha''}. \quad (39) \end{aligned}$$

$$\begin{aligned}
& \frac{-1}{\sqrt{1-x}} \sum_{G_i \in C'_-} \lim_{q \rightarrow xp_i} \tilde{\mathbf{V}}(G_i) \\
& \quad \text{Diagram: A shaded oval labeled } \tilde{\mathbf{V}}(G_i) \text{ with an incoming arrow from the top labeled } (1-x)p_i \text{ and } \alpha', \text{ and a wavy line labeled } q \text{ and } a \text{ exiting from the bottom.} \\
& = \frac{-1}{\sqrt{1-x}} \lim_{q \rightarrow xp_i} \sum_{G'_i \in C_0} \tilde{\mathbf{W}} \\
& \quad \text{Diagram: A shaded oval labeled } \tilde{\mathbf{W}} \text{ with an incoming arrow from the top labeled } (1-x)p_i \text{ and } \alpha', \text{ and a wavy line labeled } q \text{ and } a \text{ exiting from the bottom.} \\
& \quad \text{Diagram: A shaded oval labeled } \mathcal{M} \text{ with an incoming arrow from the top labeled } p_i \text{ and } \alpha''. \\
& = g_s \mu^\varepsilon T_{\alpha' \alpha''}^a \mathcal{M}
\end{aligned}$$

Fig. 2. Illustration of Eq. (39). The left hand side represents $H_{\alpha'}^a(x; p_1, \dots, p_m)$. After summing over graphs, we are left with a color matrix times the complete m particle tree amplitude.

Following the second equals sign, we have displayed the vertex at which the gluon couples to the quark line i , together with the adjacent propagator. Everything else we call $\tilde{\mathbf{W}}$. Note that $\tilde{\mathbf{W}}$ is the Green function for an amputated tree graph G'_i with m external partons. The partons have flavors $\{f_1, \dots, f_m\}$, just as with our original loop graphs, and they have the same momenta as the original partons except that parton i carries momentum $(1-x)p_i + q$. Let us denote the set of all such graphs C_0 . The sum over $G_i \in C'_-$ implies that G'_i runs over all of C_0 . In the next step, we replace q by $((1-x)p_i + q)$ next to the spinor. This gives a factor $((1-x)p_i + q)^2 / ((1-x)p_i + q)^2 = 1$. After this cancellation, it is safe to take the limit $q \rightarrow xp_i$. Also, we replace $\bar{u}((1-x)p_i)$ by $\sqrt{1-x} \bar{u}(p_i)$. In the last step, we recognize that we have the complete three level amplitude $\mathcal{M}$ for the m external particles. This calculation is illustrated in Fig. 2.

We can now insert this result into Eq. (37) and perform the loop integral to obtain

$$\begin{aligned}
\sum_{G, i \in I_C(G)} \mathcal{C}_i(G; \{p\}_m)^\alpha &= -2ig_s^2 C_F \mu^{2\varepsilon} \\
&\times \int \frac{d^d l_j}{(2\pi)^d} \frac{f_{UV}(l_j, l_j - p_i)}{(l_j^2 + i0)((p_i - l_j)^2 + i0)} \mathcal{M}(\{p\}_m)^\alpha \\
&= \frac{\alpha_s}{4\pi} C_F \frac{(4\pi)^\varepsilon}{\Gamma(1-\varepsilon)} \left(-\frac{2}{\varepsilon} + \mathcal{O}(\varepsilon) \right) \mathcal{M}(\{p\}_m)^\alpha.
\end{aligned} \tag{40}$$

Thus, when we sum over all graphs the collinear subtraction terms associated with an external quark line with label i , we get a simple singular factor times the tree level amplitude $\mathcal{M}$.

For an external antiquark line we get the same result. For an external gluon line we have a very similar result from essentially same calculation, that is

$$\sum_{G, i \in I_C(G)} \mathcal{C}_i(G; \{p\}_m) = \frac{\alpha_s}{4\pi} C_A \frac{(4\pi)^\varepsilon}{\Gamma(1-\varepsilon)} \left(-\frac{1}{\varepsilon} + \mathcal{O}(\varepsilon) \right) \mathcal{M}(\{p\}_m). \quad (41)$$

6. Final formulas

There are two steps to the algorithm that we have outlined here for generating the expressions to be used in a numerical calculation of the one-loop graphs for a QCD amplitude.

The first step applies graph by graph, generating subtractions for each graph. The subtraction terms match the integrand in the soft and collinear limits of the loop momentum. In this way, the soft and collinear divergences of the integral are removed.

The second step generates a next-to-leading order contribution to the m -parton amplitude that is proportional to the tree level matrix element (summed over tree graphs). This contribution has the form

$$I^V(\varepsilon) |\mathcal{M}_{\text{tree}}(p_1, \dots, p_m)\rangle, \quad (42)$$

where $I^V(\varepsilon)$ is a singular function of the dimensional regularization parameter ε and is a linear operator on the color space of the amplitude $|\mathcal{M}_{\text{tree}}(p_1, \dots, p_m)\rangle$. There are three parts to $I^V(\varepsilon)$. The first comes from the factors $\sqrt{r_i}$ for each external line that relate the scattering matrix to the amputated Green function. These contributions are given in Eq. (5). There is one term for each external line i . The second contribution comes from adding back the collinear subtractions. Again there is one contribution for each external line, as given in Eq. (40) for quarks and Eq. (41) for gluons. Finally, there is a third contribution that comes from adding back the soft subtractions. There is one term for each pair of external lines, as given in Eq. (22). The net result is

$$I^V(\varepsilon) = \frac{\alpha_s}{4\pi} \frac{(4\pi)^\varepsilon}{\Gamma(1-\varepsilon)} \left(\frac{1}{\varepsilon^2} \sum_{\substack{i,j=1 \\ i \neq j}}^m \mathbf{T}_i \cdot \mathbf{T}_j \left(\frac{\mu^2}{-2p_i \cdot p_j} \right)^\varepsilon - \frac{1}{\varepsilon} \sum_{i=1}^m \gamma_i \right), \quad (43)$$

where the γ_i factors are

$$\gamma_q = \gamma_{\bar{q}} = \frac{3}{2} C_F, \quad \gamma_g = \frac{11}{6} C_A - \frac{4}{6} T_R n_f. \quad (44)$$

The $1/\varepsilon^2$ and $1/\varepsilon$ poles are all of infrared origin.

We now turn to the complete calculation of an infrared safe cross section σ , which we write in the form (following as much as possible the notation of [6])

$$\sigma = \sigma_{m-n_I}^{\text{LO}} + \sigma_{m+1-n_I}^{\text{NLO}} + \sigma_{m-n_I}^{\text{NLO}}. \quad (45)$$

There are a lowest order (LO) term and two next-to-leading order (NLO) terms. We suppose that there are n_I initial state particles. (In applications, n_I is 0, 1, or 2.) The NLO term from real parton emission has $m+1-n_I$ final state particles. This is calculated from the $m+1-n_I$ particle matrix element minus subtractions. One can use, for example, the subtraction scheme proposed by Catani and Seymour [6]. The remaining NLO term has $m-n_I$ final state particles. It is calculated as follows:

$$\begin{aligned} \sigma_{m-n_I}^{\text{NLO}} = & \sum_G \int d\Phi^{m-n_I} F_J^{(m-n_I)}(\{p\}_m) \int \frac{d^4 l}{(2\pi)^4} \\ & \times 2 \operatorname{Re} \left\{ \langle \mathcal{M}_{\text{tree}}(\{p\}_m) | \tilde{\mathcal{G}}(G; \{l\}; \{p\}_m) \rangle \right. \\ & - \langle \mathcal{M}_{\text{tree}}(\{p\}_m) | \tilde{\mathcal{R}}(G; \{l\}; \{p\}_m) \rangle \\ & - \sum_{\{i,j\} \in I_S(G)} \langle \mathcal{M}_{\text{tree}}(\{p\}_m) | \tilde{\mathcal{S}}_{ij}(G; \{l\}; \{p\}_m) \rangle \\ & - \left. \sum_{i \in I_C(G)} \langle \mathcal{M}_{\text{tree}}(\{p\}_m) | \tilde{\mathcal{C}}_i(G; \{l\}; \{p\}_m) \rangle \right\} \\ & + \int d\Phi^{m-n_I} F_J^{(m-n_I)}(\{p\}_m) \\ & \times 2 \lim_{\varepsilon \rightarrow 0} \langle \mathcal{M}_{\text{tree}}(\{p\}_m) | I^V(\varepsilon) + I^R(\varepsilon) | \mathcal{M}_{\text{tree}}(\{p\}_m) \rangle. \quad (46) \end{aligned}$$

In the first term here, there is a sum over amputated one-loop graphs G . We integrate over the phase space $d\Phi$ for $m-n_I$ final state particles with momenta $p_{n_I+1}, \dots, p_m$, where the initial state particles have momenta $p_1, \dots, p_{n_I}$. Next, we supply a measurement F_J appropriate to the infrared safe observable that we wish to calculate. Then there is an integration over the loop momentum l as described in Sec. 2.1. Now there follow four terms inside the loop integration. The first is the integrand $\tilde{\mathcal{G}}$ for the graph G times the complex conjugate of the tree amplitude for $m-n_I$ final state particles. The second is $\langle \mathcal{M}_{\text{tree}} |$ times the renormalization subtraction $\mathcal{R}$, which is zero if the virtual loop graph is ultraviolet convergent. The renormalization subtraction is defined in Sec. 3. The third term contains the soft gluon subtractions $\mathcal{S}$ for graph G , one subtraction term for each pair $\{i, j\}$ of external lines that corresponds to a soft divergence. The soft subtraction is defined

in Sec. 4. The fourth term contains the collinear subtractions $\mathcal{C}$ for graph G , one subtraction term for each external line i that corresponds to a collinear divergence. The collinear subtraction is defined in Sec. 5.

There is one final term, which has no integral over a loop momentum and involves only the tree amplitude. Here we have the singular function $I^V(\varepsilon)$ from Eq. (43) that adds back the soft and collinear subtractions from the virtual graphs. We also have a singular function $I^R(\varepsilon)$ that adds back the soft and collinear subtractions from the real graphs. However, the $1/\varepsilon$ and $1/\varepsilon^2$ poles, whose structure follows from the structure of QCD, cancel between $I^V(\varepsilon)$ and $I^R(\varepsilon)$. Generally a finite contribution remains in the limit $\varepsilon \rightarrow 0$.

REFERENCES

- [1] R.K. Ellis, D.A. Ross, A.E. Terrano, *Nucl. Phys.* **B178**, 421 (1981); R.K. Ellis, J.C. Sexton, *Nucl. Phys.* **B269**, 445 (1986); Z. Bern, L.J. Dixon, D.A. Kosower, *Phys. Rev. Lett.* **70**, 2677 (1993); *Nucl. Phys.* **B437**, 259 (1995); *Nucl. Phys.* **B513**, 3 (1998); Z. Kunszt, A. Signer, Z. Trócsányi, *Phys. Lett.* **B336**, 529 (1994).
- [2] D.E. Soper, *Phys. Rev. Lett.* **81**, 2638 (1998); *Phys. Rev.* **D62**, 014009 (2000); *Phys. Rev.* **D64**, 034018 (2001); M. Kramer, D.E. Soper, *Phys. Rev.* **D66**, 054017 (2002).
- [3] T. Binoth, G. Heinrich, *Nucl. Phys.* **B585**, 741 (2000); *Nucl. Phys.* **B680**, 375 (2004); T. Binoth, G. Heinrich, N. Kauer, *Nucl. Phys.* **B654**, 277 (2003).
- [4] Z. Nagy, D.E. Soper, *J. High Energy Phys.* **09**, 055 (2003).
- [5] G. Grammer Jr., D.R. Yennie, *Phys. Rev.* **D8**, 4332 (1973); W.T. Giele, E.W.N. Glover, *D46*, 1980 (1992).
- [6] S. Catani, M.H. Seymour, *Nucl. Phys.* **B485**, 291 (1997).