Numerical calculation of one-loop integration with hypergeometric functions∗

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Abstract

One-loop two-, three- and four-point scalar functions are analytically integrated directly such that they are expressed in terms of Lauricella’s hypergeometric function $F_D$. For two- and three-point functions, exact expressions are obtained with arbitrary combination of kinematic and mass parameters in arbitrary space-time dimension. Four-point function is expressed in terms of $F_D$ up to the finite part in the expansion around 4-dimensional space-time with arbitrary combination of kinematic and mass parameters. Since the location of the possible singularities of $F_D$ is known, information about the stabilities in the numerical calculation is obtained. We have developed a numerical library calculating $F_D$ around 4-dimensional space-time. The numerical values for IR divergent cases of four-point functions in massless QCD are calculated and agreed with golem95 package.

1 Introduction

One-loop calculation in perturbative field theory is a well-established and theoretically clear method. However, highly accurate numerical calculations of one-loop amplitudes are not a trivial problem. There appear many kinematic parameters including particle masses. It is not easy to keep numerical accuracy for every points in the multi-dimensional parameter space. Since the numerical behavior of a function is related to its analytic properties, it is important to pursue stable analytical expressions for numerical calculations.

Feynman amplitudes are expected to be a kind of hypergeometric function[1]. One-loop integrals are explicitly expressed in terms of hypergeometric functions using several different methods: Mellin-Bares transformation, algebraic relations and power series expansion [2, 3, 4, 5]. See also [6] for the references. In this article, we show that one-loop two-, three- and four-point functions are directly integrated with Gauss’ function $F$, Appell’s function $F_1$ and Lauricella’s $F_D$[7]. Among these function, $F_D$ includes other functions as special cases. Since the location of possible singularities of $F_D$ is known[5], we can point out dangerous combinations of parameters and to get information about where and how numerical

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cancellation may occur. For two- or three-point functions, we show the integrals are exactly expressed in terms of $F_D$ for any values of kinematic parameters in any space-time dimensions. For four-point case, we could not integrate exactly except some special cases. However, around 4-dimensional space-time, it is expressed in terms of $F_D$ up to the finite order.

We have developed a program package which calculate $F_D$ for the necessary combinations of parameters for IR divergent case in massless QCD. We have compared our numerical result with golem95 package \[10\].

2 Two-point point function

Let’s first consider two-point scalar function as a simple example of the usage of hypergeometric function. Two-point function is defined by:

$$I^{(\alpha)}_2 = \int_0^\infty dx_1 \int_0^\infty dx_2 \frac{\delta(1 - x_1 - x_2)}{D^\alpha},$$

$$D = -p^2 x_1 x_2 + m_1^2 x_1 + m_2^2 x_2 - i\varepsilon,$$

where, $\alpha$ is a number depending on the dimension of the space-time. It is noted that calculation with arbitrary mass parameters is useful even for massless cases, since tensor integrations are obtained by differentiating scalar one in terms of mass parameters.

Integrating once with the $\delta$ function, we obtain

$$I^{(\alpha)}_2 = (m_2^2)^\alpha \int_0^1 \left(1 - \frac{x}{\gamma^+}\right)^\alpha \left(1 - \frac{x}{\gamma^-}\right)^\alpha dx,$$

$$\gamma^\pm = \frac{p^2 - m_1^2 \pm m_2^2 \pm \sqrt{D}}{2p^2}, \quad D = (-p^2 + m_1^2 + m_2^2)^2 - 4m_1^2 m_2^2.$$

This integral is nothing but a special case of Appell’s $F_1$, whose integral form is:

$$F_1(a, b, b'; c; y, z) = \frac{\Gamma(c)}{\Gamma(a) \Gamma(c - a)} \int_0^1 x^{a - 1} (1 - x)^{c - a - 1} (1 - yx)^{-b} (1 - zx)^{-b'} dx.$$ (3)

Thus we have

$$I^{(\alpha)}_2 = (m_2^2)^\alpha F_1(1, -\alpha, -\alpha; 2, \frac{1}{\gamma^+}, \frac{1}{\gamma^-}) = (m_2^2)^\alpha F_1(1, -\alpha, -\alpha; \frac{1}{1 - \gamma^+}, \frac{1}{1 - \gamma^-}).$$ (4)

The last equality is obtained by changing integration variable form $x$ to $y = 1 - x$. This equality is considered as an identity of $F_1$.

Function $F_1$ reduces to Gauss’ hypergeometric function $F$ for the case of $b' = 0$ and is a special case of more general function, called Lauricella’s $F_D$, whose integral form is:

$$F_D(a, b_1, \cdots, b_n; c; z_1, \cdots, z_n) = \frac{\Gamma(c)}{\Gamma(a) \Gamma(c - a)} \int_0^1 x^{a - 1} (1 - x)^{c - a - 1} \prod_{i=1}^n (1 - z_i x)^{-b_i} dx.$$ (5)

This function $F_D$ will be used for vertex and box integration. The location of possible singularities of $F_D$ is limited to $z_i = 0, 1, \infty$ and $z_j = z_k \ (j \neq k)$ and $F_D$ is smooth except
these special cases[8]. The power series expansion and differential equation of this function is known. Many of identities of $F$ can be generalized to $F_D$. We especially use the following identity, which can easily be confirmed from Eq.(5):

$$z^{p-1}(1-z)^{q-1} \prod_{i=1}^{n-1} (1-x_i z)^{-b_i} = \frac{dz}{dz_p} F_D(p, (b_i), 1 - q; p + 1; (x_i z), z).$$  \hspace{1cm} (6)

This identity implies that any product of linear factors with arbitrary power is integrated by $F_D$.

Now going back to Eq.(4). Two-point function $I_2^{(a)}$ may be singular when $\gamma^\pm = 0, 1, \infty$ or $\gamma^+ = \gamma^-$. These cases correspond to massless particles, $p^2 = 0$, and on the threshold. Let us examine the case of $m_2^2 = 0$ and $m_1^2, p^2 \neq 0$ for an example, where $\gamma^- = 0$ and $\gamma^+ = (p^2 - m_1^2)/p^2$. Although Eq.(4) is not well-defined for the limit of $m_2 \to 0$, we can use alternative representation obtained with another identity of $F_1$:

$$I_2^{(a)} = \frac{\gamma^-}{\alpha + 1} (m_2^2)^a F(\alpha + 1, -\alpha; \alpha + 2; \frac{\gamma^-}{\gamma^- - \gamma^+}) + \frac{1 - \gamma^-}{\alpha + 1} (m_1^2)^a F(\alpha + 1, -\alpha; \alpha + 2; \frac{1 - \gamma^-}{\gamma^+ - \gamma^-}).$$ \hspace{1cm} (7)

This representation is regular for the limit of $m_2 \to 0$ under the condition of $\Re\alpha > 0$. Then expanding around 4-dimensional space-time ($\alpha = -\epsilon \to +0$), $F_1$ is reduced to $F$ and then to log and Li$_2$. Two limiting processes $m_2 \to 0$ and $\alpha \to +0$ do not commute. This property corresponds to the fact that the analytic result in 4-dimensions does not reduce to the massless one by taking the simple limit $m_2 \to 0$.

This example shows that Eq.(4) can be used as a unified representation for both massive and massless cases. When values of mass parameters are specified, we select a suitable representation with appropriate limit. We want to select it not on a notebook but in a numerical library at the time of numerical calculations. With this library, the main program will be general to cover various cases of parameters. The problem of numerical instability will be confined into the numerical calculation method of $F_D$.

### 3 Three-point function

Three-point function is defined by:

$$I_3^{(a)} = \int_{x_1, x_2 > 0, x_1 + x_2 < 1} dx_1 \, dx_2 \, D^a. \hspace{1cm} (8)$$

where, $D$ is a quadratic form of $x_1$ and $x_2$. We apply the projective transformation as shown by Ref. [9]. The quadratic term of $x_2$ is eliminated by changing variables $(x_1, x_2) \to (x_2, z = x_1 + r x_2)$ with adjusting of the value of $r$. Since $D$ is now linear in $x_2$, integration is trivial for $x_2$. The resulting integration becomes the form:

$$I_3^{(a)} \propto \int \frac{D^{a+1}}{az + b} \, dz. \hspace{1cm} (9)$$

As $D$ is expressed as a product of linear factors of $z$, we obtain:

$$I_3^{(a)} \propto \int \frac{1}{az + b} \left(1 - \frac{z}{\gamma^+}\right)^{a+1} \left(1 - \frac{z}{\gamma^-}\right)^{\alpha+1} \, dz. \hspace{1cm} (10)$$
Using Eq. 6, this is immediately integrated by \( F \). The integration domain becomes slightly complicated after the projective transformation. It is handled systematically with exterior derivative and Stokes’ theorem. The result takes the following form:

\[
I^{(\alpha)}_3 = \frac{1}{\alpha + 1} \sum_{k=0}^{2} D_k^{\alpha+1} d_{k,1} F_{D}(1, 1, -\alpha - 1, -\alpha - 1; 2; -\frac{d_{k,1}}{d_{k,0}} \frac{1}{\gamma_k}, \frac{1}{\gamma_k})
\] (11)

where, \( D_k \) is the value of \( D \) at the corner of the integration domain and \( d_{k,j} \) is brought from the parameterization of the boundary after the projective transformation. For the limit of 4-dimensional space-time, the above expression reduces to the usual analytic representation as \( F_D \) reduces to \( F_1 \rightarrow F \rightarrow \log \) and poly-logarithmic functions.

4 Four-point function

Four-point function is written by:

\[
I^{(\alpha)}_4 = \int_{\mathbb{R}^4_{\geq 0}} d^4 x \delta \left( 1 - \sum_{j=1}^{4} x_j \right) D^{\alpha}.
\] (12)

where \( D \) is a homogeneous quadratic form of \( x_j \). After using \( \delta \) function, there left three integration variables.

We apply projective transformations twice. After the first transformation, we integrate once using the following identity:

\[
\int D^{\alpha} dy = \frac{1}{\alpha + 1} \frac{D^{\alpha+1}}{\partial_{y} D},
\] (13)

where \( D \) is quadratic in terms of remaining two variables, while \( \partial_{y} D \) is linear.

The projective transformation is applied once more. \( D \) becomes a linear function of a new variable \( z \). It is possible to select the variable \( z \) by shifting and rescaling such that \( z \propto D \) and \( 1 - z \propto \partial_{y} D \). Integral is calculated with the following formula (special case of Eq. 6):

\[
b \frac{z^{b-1}}{1-z} = \frac{\partial_{y} D}{\partial_{y} D} F(1, b; b + 1; z),
\] (14)

where \( F \) is Gauss’ hypergeometric function. After the second integration we obtain:

\[
I^{(\alpha)}_4 = \sum_{k=1}^{3} \sum_{f=1}^{4} \xi^{(4)}_k \xi^{(k)} \int_{L_{k\ell}} [g_k + h_k(e_k)] dy_{k\ell},
\] (15)

\[
g_k = \frac{1}{(\alpha + 1)(\alpha + 2)} \frac{e_k^{\alpha+1}}{d_k^{\alpha+2}} \left( \frac{d_k D_k}{e_k} \right)^{\alpha+2} F(1, \alpha + 2, \alpha + 3; \frac{d_k D_k}{e_k}),
\] (16)

where \( D_k \) and \( e_k \) are quadratic form of integration variable \( y_{k\ell} \), \( d_k \) and \( \xi^{(k)}_j \) are brought by projective transformation, and \( L_{k\ell} \) is a line segment of the last integration. Function \( h_k \) of \( e_k \) is arbitrary and is produced as an integration constant.

In order to handle \( F \) in the integrand, we use partial integration method. Using recursion relation of \( F \), \( g_k \) is expressed by:

\[
g_k = \frac{1}{(\alpha + 1)(\alpha + 2)} \frac{e_k^{\alpha+1}}{d_k^{\alpha+2}} \left( \frac{d_k D_k}{e_k} \right)^{\alpha+2}
\]

\[
+ \frac{1}{(\alpha + 1)(\alpha + 3)} \frac{e_k^{\alpha+1}}{d_k^{\alpha+2}} \left( \frac{d_k D_k}{e_k} \right)^{\alpha+3} F(1, \alpha + 3, \alpha + 4; \frac{d_k D_k}{e_k})
\] (17)
Factor $e_k^{\alpha+1}$ is integrated by the following relations:

\[
e_k(x) = \hat{e}_k(w_5 - x)(w_6 - x), \quad e_k^{\alpha+1}(x) = \frac{df(x)}{dx},
\]

\[
f(x) = \frac{1}{\alpha + 2} \frac{e_k^\alpha(x)}{\hat{e}_k(w_6 - w_5)} \left[ 1 - 2F(-\alpha - 2, \alpha + 2; \frac{w_5 - x}{w_6 - x}) \right].
\]

After the partial integration, we obtain:

\[
I_4^{(\alpha)} = \sum_{k=1,k\neq m}^{4} \sum_{\ell=1,\ell\neq k}^{4} \xi_k^{(m)} \xi_\ell^{(k)} [J_1 + J_2 + J_3],
\]

\[
J_1 = \frac{1}{(\alpha + 1)(\alpha + 2)} \int_0^1 D_k^{\alpha + 2} \frac{dx}{e_k},
\]

\[
J_2 = \frac{1}{(\alpha + 1)(\alpha + 3)} \int_0^1 \left( f(x) \left( \frac{d_k D_k}{e_k} \right)^{\alpha + 3} F(1, \alpha + 3, \alpha + 4; \frac{d_k D_k}{e_k}) \right)_{x=0},
\]

\[
J_3 = -\frac{1}{\alpha + 1} \int_0^1 f(x) \left( \frac{d_k D_k}{e_k} \right)^{\alpha + 2} \frac{d}{dx} \log \left[ \frac{e_k - d_k D_k}{e_k} \right] dx.
\]

Here we have used the following identity:

\[
\frac{d}{dx} R(x)^\alpha F(1, a + 3, a + 4; R(x)) = -(a + 3) R(x)^\alpha \frac{d}{dx} \log [1 - R(x)].
\]

\[
J_1 \text{ is integrable with } F_D, \text{ since the integrand is expressed by a product of power of linear factors. } J_2 \text{ is a product of } F. \text{ The problem left is function } f \text{ in } J_3.
\]

Investigating the limit to the 4-dimensional space-time $\alpha = -2 - \epsilon \to -2$, one will confirm that integration in $J_3$ does not produce new poles of $1/\epsilon$. So we can expand in terms of $\epsilon$ in the integrand.

\[
F(\epsilon, -\epsilon, 1 - \epsilon; z) = 1 + O(\epsilon^2).
\]

\[
J_3 = \frac{1}{\epsilon(1 + \epsilon)} \int_0^1 D_k^{\alpha + 2} \frac{d}{dx} \log \left[ \frac{e_k - d_k D_k}{e_k} \right] dx + O(\epsilon).
\]

Since factor $d \log /dx$ is expressed by a sum of inverse of linear term of $x$, $J_3$ is expressed by $F_D$ up to the finite order.

\section{5 Sample numerical calculation}

Since $F$, $F_1$ and $F_D$ have many parameters and variables, it is hard to construct numerical package to calculate for all cases. However, we need numerical values only for some special combination of parameters for our purpose.

We have tried sample numerical calculations of one-loop box tensor integration for the cases of Ref. \[4\]. That is:

- All particles are massless.
- At least one external particle is on-shell ($p_i^2 = 0$).
- Calculate up to $O(\epsilon^0)$.
• Calculate tensor integrations up to \( \text{rank} = 4 \).

There appear IR divergences, which are represented by the poles of \(1/\epsilon\).

For these cases, integration becomes simpler by using variable transformation as described in [4]. We have obtained an exact analytic representation with \( F_D \) for the cases of 4 or 3 on-shell particles and “easy case” of 2 on-shell particles (diagonal external particles of the box diagram are on-shell). However, for “hard case” of 2 on-shell particles (two adjacent external particles of the box diagram are on-shell) and 3 on-shell case, we need to expand in terms of \( \epsilon \).

It is noted that representations of \( n \)-point functions are not necessarily numerically stable when they are written with poly-logarithmic functions. For example, there appears \( F(1, m - \epsilon, m + 1 - \epsilon; z) \) \((m \geq 1)\) in the tensor integrations, which is regular around \( z \sim 0 \). When this function is expanded in terms of \( \epsilon \) using identities of \( F \), the following combination of terms appears:

\[
\frac{\epsilon^k}{z^m} \left[ \text{Li}_{k+1}(z) - \sum_{j=1}^{m-1} \frac{z^j}{j^{k+1}} \right].
\]

When \( \text{Li}_{k+1} \) is expanded around \( z \sim 0 \), the first \( m - 1 \) terms of the power series cancel out with the second term in the brackets. Factor \( z^m \) is factored out from the resulting terms in the bracket, and cancels with the denominator. If these terms are scattered into a long expression, it is not an easy problem to control these numerical cancellations and the singular behavior of the denominator. However, when we keep the original form of \( F(1, m - \epsilon, m + 1 - \epsilon; z) \), the problem is immediately solved; a simple power series calculation of \( F \) around \( z = 0 \) produces stable result. This problem is caused by the expansion made in order to express these functions in terms of \( \text{Li}_k \).

We have developed a numerical library of hypergeometric function \( F_D \) for necessary combination of parameters for our sample calculations. Our library is designed in the following way:

1. Entry points of subroutines are \( F_D \) or \( F \).
2. These subroutines return an array of coefficients of \( 1/\epsilon^2, 1/\epsilon, 1, \epsilon, \cdots \) up to necessary order.
3. Inside of the subroutines, appropriate identities or calculation methods are selected in looking at the values of parameters and variables.

Two programs are prepared for the numerical calculations of tensor integrations:

• “program-1”: calculation with numerical library of \( F, F_1 \) and \( F_D \).
• “program-2”: calculation with the following numerical integration:
  - The first two integrations are calculated analytically.
  - Coefficients of \( 1/\epsilon^2, 1/\epsilon, 1/\epsilon^0 \) are extracted and expressed by one-dimensional integrations.
  - The last integration is calculated numerically (Romberg method).
We have compared the numerical results among program-1, program-2 and golem95 package up to rank = 4 at 7560 different values of the parameters:

\[ p_1^2 = 0, \quad p_2^2 = 0, \pm 50, \quad p_3^2 = 0, \pm 55, \quad p_4^2 = 0, \pm 60, \]

\[ s = \pm 200, \quad t = \pm 123, \]

\[ n_i = 0, 1, 2, 3, 4, \quad \sum_i n_i \leq 4 \] (rank of tensor integration)

The results of the maximal differences among methods are shown by Table 1. It shows that the accuracy of the library seems similar to golem95 package.

| Calculation method | Maximal difference  |
|--------------------|---------------------|
| program-1(d)       | 7.65 \times 10^{-7} |
| program-2(d)       | 9.13 \times 10^{-10} |
| golem95(d)         | 3.98 \times 10^{-10} |
| program-1(q)       | 5.17 \times 10^{-10} |
| golem95(q)         | 1.38 \times 10^{-18} |

Table 1: Maximal differences among the calculation method. Differences are measured by the distance on the complex plane. (d) and (q) stand for double and quadruple revision respectively.

6 Summary

Two- and three-point functions are expressed in terms of \( F_D \), exactly for any combination of physical parameters in any space-time dimensions. Four-point functions are expressed with \( F_D \), up to \( O(\epsilon^0) \) for any combination of physical parameters. A program library of \( F \) and \( F_D \) is developed applicable for sample numerical calculations for massless QCD box with IR divergences. The results agree with golem95 package. Four-point function seems not to be integrated with \( F_D \). In order to express general four-point function, more general hypergeometric functions will be needed as described in [2, 3] and [11] for more general cases.

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