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Numerical calculation of one-loop integration with hypergeometric functions

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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.

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PoS(CPP2010)010

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[8], we can point out dangerous combinations of parameters and to get information about where and how numerical 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:

$$\begin{aligned} I_2^{(\alpha)} &= \int_0^\infty dx_1 \int_0^\infty dx_2\, \delta(1-x_1-x_2)\, \mathscr{D}^\alpha, \\ \mathscr{D} &= -p^2 x_1 x_2 + m_1^2 x_1 + m_2^2 x_2 - i\varepsilon, \end{aligned} \tag{2.1}$$

where, α 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 scaler one in terms of mass parameters.

Integrating once with the δ function, we obtain

$$\begin{aligned} I_2^{(\alpha)} &= (m_2^2)^\alpha \int_0^1 \left(1-\frac{x}{\gamma^+}\right)^\alpha \left(1-\frac{x}{\gamma^-}\right)^\alpha dx, \\ \mathscr{D} &= p^2x^2 + (-p^2+m_1^2-m_2^2)x + m_2^2 = m_2^2\left(1-\frac{x}{\gamma^+}\right)\left(1-\frac{x}{\gamma^-}\right), \\ \gamma^\pm &= \frac{p^2-m_1^2+m_2^2 \pm \sqrt{D}}{2p^2}, \qquad D = (-p^2+m_1^2+m_2^2)^2 - 4m_1^2m_2^2. \end{aligned} \tag{2.2}$$

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

$$F_1(a,b,b';c;y,z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 x^{a-1}(1-x)^{c-a-1}(1-yx)^{-b}(1-zx)^{-b'}\,dx. \tag{2.3}$$

Thus we have

$$I_2^{(\alpha)} = (m_2^2)^\alpha F_1(1,-\alpha,-\alpha;2;\frac{1}{\gamma^+},\frac{1}{\gamma^-}) = (m_1^2)^\alpha F_1(1,-\alpha,-\alpha;2;\frac{1}{1-\gamma^+},\frac{1}{1-\gamma^-}). \tag{2.4}$$

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:

$$F_D(a,b_1,\cdots,b_n;c;z_1,\cdots,z_n) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \int_0^1 x^{a-1}(1-x)^{c-a-1} \prod_{i=1}^{n}(1-z_i x)^{-b_i} dx. \tag{2.5}$$

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.(2.5):

$$z^{p-1}(1-z)^{q-1}\prod_{i=1}^{n-1}(1-x_i z)^{-b_i} = \frac{d}{dz}\frac{z^p}{p}F_D\left(p,(b_i),1-q;p+1;(x_i z),z\right). \tag{2.6}$$

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

Now going back to Eq.(2.4). Two-point function $I_2^{(\alpha)}$ 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.(2.4) is not well-defined for the limit of $m_2 \to 0$, we can use alternative representation obtained with another identity of F_1:

$$\begin{aligned} I_2^{(\alpha)} &= \frac{\gamma^-}{\alpha+1}(m_2^2)^\alpha F(\alpha+1,-\alpha;\alpha+2;\frac{\gamma^-}{\gamma^- - \gamma^+}) \\ &\quad + \frac{1-\gamma^-}{\alpha+1}(m_1^2)^\alpha F(\alpha+1,-\alpha;\alpha+2;\frac{1-\gamma^-}{\gamma^+ - \gamma^-}). \end{aligned} \tag{2.7}$$

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 ($\alpha = -\varepsilon \to +0$), 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-dimension does not reduces to the massless one by taking the simple limit $m_2 \to 0$.

This example shows that Eq.(2.4) 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.

PoS(CPP2010)010

3. Three-point function

Three-point function is defined by:

$$I_3^{(\alpha)} = \int_{x_1,x_2>0,x_1+x_2<1} dx_1\, dx_2\, \mathscr{D}^\alpha. \tag{3.1}$$

where, $\mathscr{D}$ 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 $(x_1,x_2) \to (x_2, z = x_1 + rx_2)$ with adjusting of the value of r. Since $\mathscr{D}$ is now linear in x_2, integration is trivial for x_2. The resulting integration becomes the form:

$$I_3^{(\alpha)} \propto \int \frac{\mathscr{D}^{\alpha+1}}{az+b}\, dz. \tag{3.2}$$

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

$$I_3^{(\alpha)} \propto \int \frac{1}{az+b}\left(1-\frac{z}{\gamma^+}\right)^{\alpha+1}\left(1-\frac{z}{\gamma^-}\right)^{\alpha+1} dz. \tag{3.3}$$

Using Eq.(2.6), this is immediately integrated by F_D. 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:

$$I_3^{(\alpha)} = \frac{1}{\alpha+1}\sum_{k=0}^{2}\frac{\mathscr{D}_k^{\alpha+1}}{a}\frac{d_{k,1}}{d_{k,0}}F_D(1,1,-\alpha-1,-\alpha-1;2;-\frac{d_{k,1}}{d_{k,0}},\frac{1}{\gamma_k^+},\frac{1}{\gamma_k^-}) \tag{3.4}$$

where, $\mathscr{D}_k$ is the value of $\mathscr{D}$ 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 $F_D \to F_1 \to F \to$ log and poly-logarithmic functions.

4. Four-point function

Four-point function is written by:

$$I_4^{(\alpha)} = \int_{\mathbb{R}^4_{\geq 0}} d^4x\, \delta\left(1-\sum_{j=1}^{4} x_j\right)\mathscr{D}^\alpha. \tag{4.1}$$

where $\mathscr{D}$ is a homogeneous quadratic form of x_j. After using δ function, there left three integration variables.

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

$$\int \mathscr{D}^\alpha dy = \frac{1}{\alpha+1}\frac{\mathscr{D}^{\alpha+1}}{\partial_y \mathscr{D}}, \tag{4.2}$$

where $\mathscr{D}$ is quadratic in terms of remaining two variables, while $\partial_y\mathscr{D}$ is linear.

The projective transformation is applied once more. $\mathscr{D}$ becomes a linear function of a new variable z. It is possible to select the variable z by shifting and rescaling such that $z \propto \mathscr{D}$ and $1-z \propto \partial_y\mathscr{D}$. Integral is calculated with the following formula (special case of Eq. (2.6)):

$$b\frac{z^{b-1}}{1-z} = \frac{d}{dz}z^b F(1,b;b+1;z), \tag{4.3}$$

where F is Gauss' hypergeometric function. After the second integration we obtain:

$$I_4^{(\alpha)} = \sum_{k=1}^{3} \sum_{\ell=1,\ell\neq k}^{4} \xi_k^{(4)} \xi_\ell^{(k)} \int_{L_{k\ell}} [g_k + h_k(e_k)]\, dy_{k\ell}, \tag{4.4}$$

$$g_k = \frac{1}{(\alpha+1)(\alpha+2)} \frac{e_k^{\alpha+1}}{d_k^{\alpha+2}} \left(\frac{d_k \mathscr{D}_k}{e_k}\right)^{\alpha+2} F(1,\alpha+2,\alpha+3;\frac{d_k\mathscr{D}_k}{e_k}), \tag{4.5}$$

where $\mathscr{D}_k$ and e_k are quadratic form of integration variable y_{kl}, d_k and $\xi_\ell^{(k)}$ 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:

$$\begin{aligned} g_k = &\frac{1}{(\alpha+1)(\alpha+2)} \frac{e_k^{\alpha+1}}{d_k^{\alpha+2}} \left(\frac{d_k \mathscr{D}_k}{e_k}\right)^{\alpha+2} \\ &+ \frac{1}{(\alpha+1)(\alpha+3)} \frac{e_k^{\alpha+1}}{d_k^{\alpha+2}} \left(\frac{d_k \mathscr{D}_k}{e_k}\right)^{\alpha+3} F(1,\alpha+3,\alpha+4;\frac{d_k\mathscr{D}_k}{e_k}) \end{aligned} \tag{4.6}$$

Factor $e_k^{\alpha+1}$ is integrated by the following relations:

$$\begin{aligned} &e_k(x) = \tilde{e}_k\,(w_5 - x)(w_6 - x), \qquad e_k^{\alpha+1}(x) = \frac{df(x)}{dx}, \\ &f(x) = \frac{1}{\alpha+2} \frac{e_k^{\alpha+2}(x)}{\tilde{e}_k(w_6-w_5)} \Big[1 - 2F(-\alpha-2,\alpha+2,\alpha+3;\frac{w_5-x}{w_6-x})\Big]. \end{aligned} \tag{4.7}$$

After the partial integration, we obtain:

$$\begin{aligned} I_4^{(\alpha)} &= \sum_{k=1,k\neq m}^{4} \sum_{\ell=1,\ell\neq k}^{4} \xi_k^{(m)} \xi_\ell^{(k)} [J_1 + J_2 + J_3], \\ J_1 &= \frac{1}{(\alpha+1)(\alpha+2)} \int_0^1 \frac{\mathscr{D}_k{}^{\alpha+2}}{e_k}\, dx, \\ J_2 &= \frac{1}{(\alpha+1)(\alpha+3)} \frac{1}{d_k^{\alpha+2}} \Big[f(x) \left(\frac{d_k\mathscr{D}_k}{e_k}\right)^{\alpha+3} F(1,\alpha+3,\alpha+4;\frac{d_k\mathscr{D}_k}{e_k})\Big]_{x=0}^{1}, \\ J_3 &= -\frac{1}{\alpha+1} \frac{1}{d_k^{\alpha+2}} \int_0^1 f(x) \left(\frac{d_k\mathscr{D}_k}{e_k}\right)^{\alpha+2} \frac{d}{dx} \log\left[\frac{e_k - d_k\mathscr{D}_k}{e_k}\right] dx. \end{aligned} \tag{4.8}$$

Here we have used the following identity:

$$\frac{d}{dx} R(x)^{a+3} F(1,a+3,a+4;R(x)) = -(a+3)R(x)^{a+2} \frac{d}{dx} \log[1-R(x)]. \tag{4.9}$$

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

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

$$F(\varepsilon,-\varepsilon,1-\varepsilon;z) = 1+\mathscr{O}(\varepsilon^2). \tag{4.10}$$

$$J_3 = \frac{1}{\varepsilon(1+\varepsilon)}\frac{1}{\tilde{e}_k(w_6-w_5)}\int_0^1 \mathscr{D}_k{}^{\alpha+2}\frac{d}{dx}\log\left[\frac{e_k-d_k\mathscr{D}_k}{e_k}\right]dx+\mathscr{O}(\varepsilon). \tag{4.11}$$

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.

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 ($p_1^2 = 0$).
- Calculate up to $\mathscr{O}(\varepsilon^0)$.
- Calculate tensor integrations up to rank $= 4$.

There appear IR divergences, which are represented by the poles of $1/\varepsilon$.

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 ε.

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 $F(1,m-\varepsilon,m+1-\varepsilon;z)$ $(m\geq 1)$ in the tensor integrations, which is regular around $z\sim 0$. When this function is expanded in terms of ε using identities of F, the following combination of terms appears:

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

When 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 $F(1,m-\varepsilon,m+1-\varepsilon;z)$, 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 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:

PoS(CPP2010)010

1. Entry points of subroutines are F_D or F.
2. These subroutines return an array of coefficients of $1/\varepsilon^2, 1/\varepsilon, 1, \varepsilon, \cdots$ 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 $1/\varepsilon^2, 1/\varepsilon^1, 1/\varepsilon^0$ 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:

$$p_1^2 = 0, \qquad p_2^2 = 0, \pm 50, \qquad p_3^2 = 0, \pm 55, \qquad p_4^2 = 0, \pm 60,$$
$$s = \pm 200, \qquad t = \pm 123,$$
$$n_i = 0,1,2,3,4, \qquad \sum_i n_i \leq 4 \qquad \text{(rank of tensor integration)}$$

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)	program-2(d)	7.65×10^{-7}
program-1(d)	`golem95` (d)	9.13×10^{-10}
program-1(d)	program-1(q)	3.98×10^{-10}
`golem95`(d)	`golem95`(q)	5.17×10^{-10}
program-1(q)	`golem95` (q)	1.38×10^{-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 recision 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 $\mathscr{O}(\varepsilon^0)$ 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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