BOKASUN: a fast and precise numerical program to calculate the Master Integrals of the two-loop sunrise diagrams.  

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Abstract

We present the program BOKASUN for fast and precise evaluation of the Master Integrals of the two-loop self-mass sunrise diagram for arbitrary values of the internal masses and the external four-momentum. We use a combination of two methods: a Bernoulli accelerated series expansion and a Runge-Kutta numerical solution of a system of linear differential equations.

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Key words: Feynman diagrams, sunrise diagram, numerical evaluation

PROGRAM SUMMARY

Program Title: BOKASUN
Journal Reference:  
Catalogue identifier:  
Licensing provisions: none  
Programming language: FORTRAN77  
Computer: any computer with FORTRAN compiler accepting FORTRAN77 standard; tested on various PC's with LINUX  
Operating system: LINUX  
RAM: 120 kbytes  
Classification: 4.4

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Nature of problem:
Any integral arising in the evaluation of the two-loop sunrise Feynman diagram can be expressed in terms of a given set of Master Integrals, which should be calculated numerically. The program provides with a fast and precise evaluation method of the Master Integrals for arbitrary (but not vanishing) masses and arbitrary value of the external momentum.

Solution method:
The integrals depend on three internal masses and the external momentum squared $p^2$. The method is a combination of an accelerated expansion in $1/p^2$ in its (pretty large!) region of fast convergence and of a Runge-Kutta numerical solution of a system of linear differential equations.

Running time:
To obtain 4 Master Integrals on PC with 2 GHz processor it takes 3 $\mu$s for series expansion with calculated in advance coefficients, 80 $\mu$s for series expansion without calculated in advance coefficients, from few seconds up to few minutes for Runge-Kutta method (depending on the required accuracy and the values of the physical parameters).

LONG WRITE-UP

1 Introduction

The sunrise diagram with arbitrary masses is one of the basic ingredients of any two-loop calculation, and its fast numerical evaluation is of direct interest in Monte Carlo simulation programs. Many procedures for a precise evaluation of the Master Integrals (MI’s) can be found in the literature [1,2,3,4,5,6,7,8,9,10,11,12,13,14]. In [15] a fast and precise series expansion was proposed in the much simpler case of equal internal masses. In this paper we adapt the method to the arbitrary mass case by considering the accelerated expansion in inverse powers of $p^2$, which provides with a fast and precise convergence in a wide region covering the biggest part of $p^2$ values. The expansion does not work in a relatively small region (roughly from $p^2 = 0$ to the physical threshold). A similar expansion in $p^2$ around the regular point $p^2 = 0$ (the first terms where given in [16]) is unpractical due to the severe numerical instability of the coefficients of the expansion [17], associated with the presence of nearby pseudothresholds (this feature is peculiar to the arbitrary mass case, as opposed to the equal mass limit). In the regions were the expansion in $1/p^2$ does not work we use the Runge-Kutta algorithm developed in [11,18,19] to obtain the Master Integrals (MI’s) of the sunrise diagram as the numerical solutions of a suitable system of linear differential equations. The execution
time is of the order of a few seconds (minutes) when the Runge-Kutta method is used (depending on the values of \( p^2 \) and the masses and also on the required precision), while it drops to about 80 \( \mu s \) when the new expansion applies and to 3 \( \mu s \) if the expansion coefficients are calculated in advance (all CPU times are given for a 2 GHz PC).

2 The notation

We use here the same notation and definitions as in [11], which we recall shortly for convenience of the reader. The four Master Integrals (MI’s) related to the general massive 2-loop sunrise self-mass diagram in \( n \) continuous dimensions and with fully Euclidean variables are defined as

\[
F_j(n, m_1^2, m_2^2, m_3^2, p^2) = \frac{\mu^{8-2n}}{(2\pi)^{n-2}} \int d^n k_1 \int d^n k_2 \frac{1}{(k_1^2 + m_1^2)^{\alpha_1(j)}(k_2^2 + m_2^2)^{\alpha_2(j)}((p - k_1 - k_2)^2 + m_3^2)^{\alpha_3(j)}},
\]

(1)

where \( j = 0, 1, 2, 3 \) refers to the 4 MI’s; for \( j = 0 \), \( \alpha_i(j = 0) = 1 \) for \( i = 1, 2, 3 \); for \( j > 0 \), \( \alpha_i(j) = 2 \) when \( i = j \) and \( \alpha_i(j) = 1 \) when \( i \neq j \).

The mass scale is chosen as

\[
\mu = m_1 + m_2 + m_3 ,
\]

(2)

which comes out to be the appropriate mass scale parameter for the numerical discussion. The expansion of the MI’s around \( n = 4 \) has the form [16]

\[
F_j(n, m_1^2, m_2^2, m_3^2, p^2) = C^2(n) \left\{ \frac{1}{(n-4)^2} F_j^{(-2)}(m_1^2, m_2^2, m_3^2, p^2) \right. \\
+ \left. \frac{1}{(n-4)} F_j^{(-1)}(m_1^2, m_2^2, m_3^2, p^2) + F_j^{(0)}(m_1^2, m_2^2, m_3^2, p^2) + O(n-4) \right\} ,
\]

(3)

where the coefficient \( C(n) \)

\[
C(n) = \left( 2\sqrt{\pi} \right)^{(4-n)} \Gamma \left( 3 - \frac{n}{2} \right) ,
\]

(4)
not to be expanded, can be replaced by its value $C(4) = 1$, at $n = 4$, when multiplying a function regular in $(n - 4)$. The coefficients of the poles in $(n - 4)$ of $F_j(n, m_1^2, m_2^2, m_3^2, p^2)$ are known in closed analytic form [16,11], and are not reconsidered here, as from now on we deal only with the finite parts $F_j^{(0)}(m_1^2, m_2^2, m_3^2, p^2)$ of the MI's.

It is convenient to use reduced masses and reduced external invariant

$$m_{i,r} \equiv \frac{m_i}{m_1 + m_2 + m_3}, \quad p_r^2 \equiv \frac{p^2}{(m_1 + m_2 + m_3)^2},$$

(5)
together with a dimensionless version of $F_0(n, m_1^2, m_2^2, m_3^2, p^2)$, defined by

$$F_{0,r}(n, m_1^2, m_2^2, m_3^2, p^2) \equiv \frac{F_0(n, m_1^2, m_2^2, m_3^2, p^2)}{(m_1 + m_2 + m_3)^2};$$

(6)
as the other Master Integrals are already dimensionless, the values of all the functions are also dimensionless. In terms of the new variables $p_r^2, m_{i,r}$ the threshold is located at $p_{th,r}^2 = -1$.

Moreover we do not write anymore, for short, the arguments of the functions and the superscript $(0)$, so we set $F_0 \equiv F_{0,r}(m_1^2, m_2^2, m_3^2, p^2)$ and $F_j \equiv F_j^{(0)}(m_1^2, m_2^2, m_3^2, p^2), \; j = 1, 2, 3$.

### 3 Handling of the asymptotic expansion

The asymptotic expansion at large $p_r^2$ values was proposed in [16], but only few terms were given there explicitly. It can be written symbolically as

$$F_i = \Sigma_{i,0} + \log(p_r^2)(\Sigma_{i,1}) + \log^2(p_r^2)(\Sigma_{i,2}), \quad i = 0, 1, 2, 3,$$

(7)
where $\Sigma_{i,j}$ are power series in $1/p_r^2$. For the purpose of the program presented here, up to 18 terms in inverse powers of $p_r^2$ were evaluated. That required the solution of a system of four linear equations per set of coefficients. Each coefficient in the expansion is a polynomial in three masses and logarithms of the masses. As the length of the coefficients is growing with the growing inverse power of $p_r^2$ we have made an effort to shorten the expressions using symmetric polynomials for $F_0$. The polynomials are calculated once and used several times in the evaluation of the coefficients. For the $F_i \; (i = 1, 2, 3)$ we found out that the most effective way to simplify the coefficients is to make use of the relation $F_i(n, m_1^2, m_2^2, m_3^2, p^2) = -\partial F_0(n, m_1^2, m_2^2, m_3^2, p^2)/\partial m_i^2$ after the
simplification of the coefficients of $F_0$. All that resulted not only in shortening of the expressions, but what is more important, in significant (about 10 times) gain in CPU time necessary for the calculation of the sunrise master integrals.

To speed up the convergence of the series and to enlarge the convergence region we use the Bernoulli change of variables, introduced in [20] and systematically used in [21,15], separately for each of the series $\Sigma_{i,j}$ from Eq.(7). Each of the series $\Sigma$ (we drop here the subscript to shorten the expressions)

\[ \Sigma = \sum_{n=0}^{\infty} a_n \left( \frac{1}{p^2} \right)^n, \] (8)

after the (Bernoulli) change of variable

\[ y = \log \left( 1 + \left( \frac{1}{p^2} \right) \right) \] (9)

becomes

\[ \Sigma = a_0 + \sum_{l=0}^{\infty} \frac{1}{l!} y^l b_l, \] (10)

with

\[ b_l = \sum_{n=1}^{l} a_n (-1)^n \sum_{k=0}^{n} \frac{n!}{(n-k)!k!} (-1)^k k^l. \] (11)

We obtain an expansion in $y$ which, with 18 terms, provides with double precision (real*8) results for all values of $p^2_r$ outside the interval $[-1.5,0.5]$ and for arbitrary masses. The precision of the result is estimated by taking the ratio of the last term to the sum of all the terms. As a matter of fact the double precision accuracy is obtained for particular values of masses also in a wider region of $p^2_r$ (see next section). The estimation of the error was checked against the results of a Runge-Kutta method of comparable precision. It is to be recalled here that the convergence of the expansion in powers of $1/p^2_r$ is superior to the Runge-Kutta approach for large values of $p^2_r$, so that the check is a really stringent one in the region $-1.5 < p^2_r < -1$ and $0 < p^2_r < 0.5$ at the borderline of the convergence of the expansion.

As the coefficients of the Bernoulli accelerated series are obtained numerically, we have checked the numerical stability of the procedure. The expected cancellations occurring in Eq.(11) were never affecting the accuracy of the result.
and the formulae remained numerically stable at variance with the formulae for the expansion at $p^2 = 0$, which were thus not used in the program.

For the values of $p^2_r$ for which the asymptotic expansion does not work we use the direct numerical solution of the system of differential equations by means of the Runge-Kutta method described in details in [11]. The algorithm works relatively fast in the region of small $p^2_r$ values. Thus the combination of the methods, used in the present program, allows for the fast and accurate evaluation of the sunrise Master Integrals for all values of $p^2_r$.

4 The outline of the program

The way the program works is shown schematically in Fig. 1. First, the program reads from the file input.BOKASUN.dat the values of $p^2, m_1, m_2, m_3$, the required relative accuracies (denoted as $\Delta_r$, $\Delta_r = (\text{acc}(1), \text{acc}(2), \text{acc}(3))$) for the real parts, the imaginary parts and the moduli of the four functions, which the user wishes to calculate. The program checks if the value of the squared rescaled four momentum ($p^2_r$) is within the interval $A = [-1, 0]$, where the series expansion is not valid. For $p^2_r \in A$ the program uses the Runge-Kutta method, described in [11], and gives the values of all functions $F_n$. The program tries to reach the accuracy asked by the user and gives the values with the best obtained accuracy, even if the required accuracy was not reached. Outside the interval $A$ the program evaluates first the value of the functions $F_n$ by using the asymptotic expansion described in the previous section. If the estimated relative accuracies for real and imaginary parts are lower than $10^{-14}$ or the accuracies are better (or equal) than (to) the accuracies asked by the user the program writes the $F_n$ with their relative accuracies for real and imaginary parts. If any of the accuracy requirements is not met the program uses Runge-Kutta method to calculate all functions $F_n$, $n = 0, 1, 2, 3$. The result with better accuracy is written as the output.

There are two subroutines to calculate the MI’s:

bokasun, where the series expansion coefficients are calculated for each call, and

bokasun_s, where the series expansion coefficients are calculated in advance in the subroutine prepare_store

The second option is useful when one needs to calculate the MI’s for fixed masses and various $p^2$ values. It speeds up the calculations about 25 times.

Both subroutines are called with parameters:
Fig. 1. The flowchart of the BOKASUN program (see the text for details). $\Delta_s$ ($\Delta_{rk}$): accuracy obtained by the expansion (Runge-Kutta) method. $F_n^s$ ($F_n^{rk}$), $n = 0, \ldots, 3$: results obtained by means of the expansion (Runge-Kutta) method. The $\Delta_s < \Delta_{rk}$ condition is checked separately for the real and the imaginary part of each MI. Thus, when the MI's are calculated by both methods, the result with better accuracy is given in the output.

\begin{verbatim}
p2,m1in,m2in,m3in,acc,Fn,deltare,deltaim
\end{verbatim}

declared as

\begin{verbatim}
real*8 p2,m1in,m2in,m3in,acc(3)
complex*16 Fn(0:3)
real*8 deltare(0:3),deltaim(0:3)
\end{verbatim}
p2 is the square of the four momentum

m1in, m2in, m3in are the internal masses

acc(1) is the required relative precision for the real parts of the MI's

acc(2) is the required relative precision for the imaginary parts of the MI's

acc(3) is the required relative precision for the modulus of the MI's; used only for Runge-Kutta method

Fn(i), i=0,1,2,3 finite part of the ith MI

deltare(i) (deltaim(i)) relative accuracy of the real (imaginary) part of the ith MI

5 Tests of the program and typical run times

In [11] many tests of the Runge-Kutta method were performed in all regions of the $p^2$ values. Comparisons have shown an excellent agreement between the code developed in [11] and the values published in [1,8]. In [12] the author states also the complete agreement with [11] of his code, published later as a part of [14]. In view of these comparisons we have just checked that the new part of the program, which uses the large $p^2_r$ expansion gives results which are in agreement with the Runge-Kutta method. As matter of fact, when the expansion in $1/p^2_r$ applies, our program reaches a precision of $10^{-14}$ or better, which is higher than the other available programs, so that a direct comparison up to that precision was in general not possible. Nevertheless, extensive comparisons were made, limited to the relative precision of $10^{-11}$ (or slightly better; that is the maximum precision which one can reach with the Runge-Kutta method for large $p^2_r$ values) for various sets of masses. The results were always in agreement within the errors. Machine precision comparisons were possible with [15] in the equal mass case, and an excellent agreement was found.

The main gain in using the series expansion, whenever possible, is the reduction of CPU time necessary to obtain the result. The CPU time (on a laptop with Intel Centrino Duo T7400 2.16 GHz processor) necessary for calculation of the Master Integrals with the double precision machine accuracy, with the expansion method, is about $8 \cdot 10^{-5}$ s, which reduces to about $3 \cdot 10^{-6}$ s when the expansion coefficients are calculated in advance. With the Runge-Kutta method it takes 10 s at $p^2_r = 0.1$ and 1800 s at $p^2_r = 10$ to obtain the relative accuracy of $10^{-11}$. 

8
TEST RUN OUTPUT

The distributed version of the program contains also a code of the test run, which uses both subroutines bokasun and bokasun.s. It provides also with an example of using the BOKASUN program. It reads the input parameters for the test run from the file input_BOKASUN.dat and appends the results of the MI’s with the obtained relative accuracies to files f0.dat (F0), f1.dat (F1), f2.dat (F2) and f3.dat (F3). In the files f0.dat.ref, f1.dat.ref, f2.dat.ref and f3.dat.ref, distributed together with the program, the results expected for the test run are given. The test run takes about 6 minutes CPU as it calculates many points using the Runge-Kutta method.

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