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Harmonic sums, Mellin transforms and Integrals

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Abstract

This paper describes algorithms to deal with nested symbolic sums over combinations of harmonic series, binomial coefficients and denominators. In addition it treats Mellin transforms and the inverse Mellin transformation for functions that are encountered in Feynman diagram calculations. Together with results for the values of the higher harmonic series at infinity the presented algorithms can be used for the symbolic evaluation of whole classes of integrals that were thus far intractable. Also many of the sums that had to be evaluated seem to involve new results. Most of the algorithms have been programmed in the language of FORM. The resulting set of procedures is called SUMMER.

1 Introduction

The computation of Feynman diagrams has confronted physicists with classes of integrals that are usually hard to be evaluated, both analytically and numerically. Also the newer techniques applied in the more popular computer algebra packages do not offer much relief. Therefore it is good to occasionally study some alternative methods to come to a result. In the case of the computation of structure functions in deep inelastic scattering one is often interested in their Mellin moments. Each individual moment can be computed directly in ways that are much easier than computing the whole structure function and taking its moments afterwards. There exist however also instances in the literature in which all moments were evaluated in a symbolic way [1] [2] [3] [4]. Once all positive even moments are known, one can reconstruct the complete structure functions. Hence such calculations contain the full information and are in principle as valuable as the direct evaluation of the complete integrals. In these calculations the integrals become much simpler at the cost of having to do a number of symbolic sums over harmonic series. The draw-back of the method is that although much effort has been put in improving techniques of integration over the past years, very little is known about these classes of sums. A short introduction is given for instance in ref [5]. In addition such calculations are of a nature that one needs to do them usually by means of a computer algebra program. This means that when algorithms are developed, they should be suitable for implementation in the language of such programs.

This paper describes a framework in which such calculations can be done. As such it gives a consistent notation that is suited for a computer program. It shows a number of sums that can be handled to any level of complexity and describes an implementation of them in the language of the program FORM [6]. Then the formalism is applied to the problem of Mellin transforms of a class of functions that traditionally occurs in the calculation of Feynman diagrams. This in its turn needs harmonic series in infinity and hence there is a section on this special case. Next the problem of the inverse Mellin transform is dealt with. With the results of the series at infinity one can suddenly evaluate a whole class of integrals symbolicaly. This is explained in the next section where some examples are given.

The paper is finished with a number of appendices. They describe the details of some of the algorithms and their implementation. Additionally there is an appendix with lists of symbolic sums that are not directly treated by the 'general' algorithms. These sums were obtained during various phases of the project and many of them do not seem to occur in the literature.

2 Notations

The notation that is used for the various functions and series in this paper is closely related to how useful it can be for a computer program. This notation stays as closely as possible to existing ones. The harmonic series is defined by

$$S_m(n) = \sum_{i=1}^{n} \frac{1}{i^m} \tag{1}$$

$$S_{-m}(n) = \sum_{i=1}^{n} \frac{(-1)^i}{i^m} \tag{2}$$

in which $m > 0$. One can define higher harmonic series by

$$S_{m,j_1,\cdots,j_p}(n) = \sum_{i=1}^{n} \frac{1}{i^m} S_{j_1,\cdots,j_p}(i) \tag{3}$$

$$S_{-m,j_1,\cdots,j_p}(n) = \sum_{i=1}^{n} \frac{(-1)^i}{i^m} S_{j_1,\cdots,j_p}(i) \tag{4}$$

with the same conditions on m. The m and the j_i are referred to as the indices of the harmonic series. Hence

$$S_{1,-5,3}(n) = \sum_{i=1}^{n} \frac{1}{i} \sum_{j=1}^{i} \frac{(-1)^j}{j^5} \sum_{k=1}^{j} \frac{1}{k^3} \tag{5}$$

In the literature the alternating sums are usually indicated by a bar over the index. The advantage of this notation is that it can be extended easily for use in a computer algebra program, eg.:

$$S_{i_1,\cdots,i_m}(n) \rightarrow \texttt{S(R(i1,...,im),n)}.$$

Such objects can be easily manipulated in the more modern versions of the program FORM.

The argument of a harmonic series which has only positive indices can be doubled with the formula:

$$S_{m_1,\cdots,m_p}(n) = \sum_{\pm} 2^{m_1+\cdots+m_p-p} S_{\pm j_1,\cdots,\pm j_p}(2n) \tag{6}$$

in which the sum is over all 2^p combinations of $+$ and $-$ signs.

The weight of a harmonic series is defined as the sum of the absolute values of its indices.

$$W(S_{j_1,\cdots,j_m}(n)) = \sum_{i=1}^{m} |j_i| \tag{7}$$

For any positive weight w there are $2 \times 3^{w-1}$ linearly independent harmonic series. The fact that for each next weight there are three times as many can be seen easily: One can extend the series of the previous weight either by putting an extra index 1 or -1 in front, or by raising the absolute value of the first index by one.

The set of all harmonic series with the same weight is called the 'natural' basis for that weight.

The extended weight of the compound object of a series and denominators is the weight of the series plus the number of powers of denominators that are identical to the argument of the series. Hence $S_{1,-5,3}(n)/n^4$ has the extended weight 13.

The total weight of a term is the sum of all extended weights of all the series in that term. Hence the total weight of $S_{2,3}(n)S_{-2}(m)$ is 7.

The value 0 for an index is reserved for an application that is typical for computers. If the results of a given weight need to be tabulated, the above notation would require a table in which the number of indices is not fixed. This can be remedied by a modified notation which is only used in specific stages of the program. An index that is zero which is followed by an index that is nonzero indicates that one should be added to the absolute value of the nonzero index. Hence:

$$S_{0,1,0,0,-1,1}(n) = S_{2,-3,1}(n) \tag{8}$$

This way one can express all series of weight w into functions with w indices of which the first $w-1$ can take the values 1, 0 and -1, while the last one can take the values 1 and -1.

Consider the following identity which can be obtained by exchanging the order of summation:

$$S_{j,k}(n) + S_{k,j}(n) = S_j(n)S_k(n) + S_{j\&k}(n) \tag{9}$$

in which the pseudo addition operator & adds the absolute values and gives the result a positive value if j and k have the same sign and otherwise the result will have a negative value. One could select a basis in which one keeps products of harmonic series with as simple a weight as possible. The above equation would indicate that in that case one of the left terms should be excluded from the basis in favor of the first term on the right hand side. Although the choice of which of the higher harmonic series to keep and which to drop in favor of the product terms is not unique, there are cases in which such a basis is to be preferred. In particular when $n \to \infty$ one can choose a basis in which all divergent objects are expressed as powers of $S_1(\infty)$ multiplied by finite harmonic series. In general however the summation formulae are much simpler in the natural basis in which each element is a single higher harmonic series. This can be seen rather easily when looking at the sum:

$$\begin{aligned}\sum_{i=1}^{n} \frac{S_j(i)S_k(i)}{i^m} &= \sum_{j=1}^{n} \frac{S_{j,k}(i)+S_{k,j}(i)-S_{j\&k}(i)}{i^m} \\ &= S_{m,j,k}(n)+S_{m,k,j}(n)-S_{m,j\&k}(n) \qquad (10)\end{aligned}$$

In order to be able to do the sum one has to convert to the natural basis anyway. After the summation one would have to convert back to whatever other basis one happens to work with. Appendix A presents an algorithm by which combinations of harmonic series with the same argument can be expressed in the natural basis.

Additionally there can be denominators containing the summation parameter. There arises immediately a problem when there is more than one denominator. Traditionally one can split the fractions with

$$\frac{1}{i+a}\frac{1}{i+b} = \frac{1}{b-a}\left(\frac{1}{i+a}-\frac{1}{i+b}\right) \qquad (11)$$

Unfortunately this formula is not correct when $a = b$. Because often there will be nested sums and sums with symbolic parameters, a and b can be functions of summation or other parameters and hence it will not be obvious when $a = b$. In FORM this can be repaired in principle with one of the special functions:

$$\frac{1}{i+a}\frac{1}{i+b} = \delta_{a,b}\frac{1}{(i+a)^2} + (1-\delta_{a,b})\frac{1}{b-a}\left(\frac{1}{i+a}-\frac{1}{i+b}\right) \qquad (12)$$

Here $\delta_{a,b} = 1$ when $a = b$ and zero otherwise. In the language of FORM it is represented by the built in object `delta_`. Unfortunately this form of the partial fractioning is not very useful, because it still evaluates into terms involving 1/(b-a) in which a can be equal to b. Hence an even more complicated form is needed:

$$\frac{1}{i+a}\frac{1}{i+b} = \delta_{a,b}\frac{1}{(i+a)^2} + (\theta(a-b-1)+\theta(b-a-1))\frac{1}{b-a}\left(\frac{1}{i+a}-\frac{1}{i+b}\right) \qquad (13)$$

in which one has to assume that a and b only take integer values. The function $\theta(x)$ (in FORM `theta\_(x)`) is zero when x is negative and one when x is zero or positive. These θ-functions fulfill the rôle of conditions like $a \geq b+1$ plus $b \geq a+1$ and are worked out first. Hence this should not be read as 0/0 for the case that $a = b$. The complete and proper equation would involve a new function:

$$\frac{1}{i+a}\frac{1}{i+b} = \delta_{a,b}\frac{1}{(i+a)^2} + (\theta'(a-b)+\theta'(b-a))\frac{1}{b-a}\left(\frac{1}{i+a}-\frac{1}{i+b}\right) \qquad (14)$$

with $\theta'(x)$ (in FORM `thetap\_(x)`) is one when $x > 0$ and zero when $x \leq 0$. Actually $\theta'(x) = 1-\theta(-x)$, but this cannot be used for the same reason that the equation (12) could not be used. Because it is rather complicated to manipulate both the functions $\theta(x)$ and $\theta'(x)$ simultaneously, and because one has almost always integer values of the parameter, the computer program uses mostly the formula (13) which assumes the integer values. It should be clear that much attention should be given to theta and delta functions, their combinations and their interactions with summations.

3 Synchronization

When one has to do sums over a combination of objects one of the problems is that such objects do not always have identical arguments. If this is the case one would have to program many more sums than often is necessary. Whenever it is possible one should ‘synchronize’ the arguments. This means that one tries to make the arguments of the various harmonic series, the denominators and the factorials equal to each other. This can be illustrated with one harmonic series and one denominator:

$$\begin{aligned}\sum_{i=1}^{n}\frac{S_1(i+1)}{i} &= \sum_{i=1}^{n}\frac{S_1(i)}{i}+\sum_{i=1}^{n}\frac{1}{i+1}\frac{1}{i}\\ &= \sum_{i=1}^{n}\frac{S_1(i)}{i}+\sum_{i=1}^{n}\frac{1}{i}-\sum_{i=1}^{n}\frac{1}{i+1}\end{aligned} \tag{15}$$

In this equation and the sequel it is assumed that the left most index is positive. If it is negative there will be the extra $(-1)^i$ and one has to be more careful with the signs of the terms, but the principle is always the same.

Of course, when the difference between some arguments is symbolic like in $S_1(i+k)/i$, such tricks do not work, but for differences that are integer constants one can define a scheme that converges. Let m be a positive integer constant in the remaining part of this section. In that case one can write:

$$\frac{S_{j,r_1,\cdots,r_s}(i+m)}{i} = \frac{S_{j,r_1,\cdots,r_s}(i+m-1)}{i}+\frac{S_{r_1,\cdots,r_s}(i+m)}{i(i+m)^j} \tag{16}$$

The partial fractioning of the denominators in the last term results in terms that have only a power of $1/(i+m)$ and one term which has a factor $1/i$. This last term however has a simpler harmonic series in the numerator. Hence this relation defines a recursion that terminates. Similarly one can write:

$$\frac{S_{j,r_1,\cdots,r_s}(i)}{i+m} = \frac{S_{j,r_1,\cdots,r_s}(i+1)}{i+m}-\frac{S_{r_1,\cdots,r_s}(i+1)}{(i+m)(i+1)^j} \tag{17}$$

and partial fractioning results again in terms in which the arguments either are the same, or closer to each other, or the harmonic series has become simpler.

Next is the interaction between two harmonic series:

$$\begin{aligned}S_{j,r_1,\cdots,r_s}(i)S_{p_1,\cdots,p_q}(i+m) &= S_{j,r_1,\cdots,r_s}(i+1)S_{p_1,\cdots,p_q}(i+m)\\ &\quad -S_{r_1,\cdots,r_s}(i+1)S_{p_1,\cdots,p_q}(i+m)\frac{1}{(i+1)^j}\end{aligned} \tag{18}$$

This relation defines, in combination with the previous two equations, also a proper recursion. In the last term one can synchronize the argument of the second harmonic series with that of the denominator, giving (potentially many) terms with either $1/(i+m)$ or an argument that is closer to $i+1$. In all cases the arguments are at least one closer to each other. In addition some of the harmonic series have become simpler.

Once two harmonic series have the same arguments this product can be rewritten into the basis of single higher harmonic series (see appendix A). Hence products of more than two harmonic series with different arguments can be dealt with successively.

At this point there can still be factorials. The beginning is easy:

$$\begin{aligned}\frac{1}{i\ (i+m)!} &= \frac{1}{i\ (i+m)\ (i+m-1)!}\\ &= \frac{1}{m}\frac{1}{i\ (i+m-1)!}-\frac{1}{m}\frac{1}{(i+m)!}\end{aligned}\tag{19}$$

and

$$\begin{aligned}\frac{1}{(i+m)\ i!} &= \frac{i+1}{(i+m)\ (i+1)!}\\ &= \frac{1}{(i+1)!}-\frac{m-1}{(i+m)\ (i+1)!}\end{aligned}\tag{20}$$

Because of these two equations one can also synchronize combinations of harmonic series and factorials.

The problem is that usually one cannot do very much with the product of two factorials. This means that if one has more than one factorial, one may be left with factorials with different arguments.

Another problem exists with arguments of the type i versus arguments of the type $n-i$. These can of course not be synchronized completely, but if n is the upper limit of the summation over i, one can try to make a synchronization that excludes other nonsymbolic constants. This is slightly more complicated than what was done before:

$$\frac{1}{n-i}S_{j,r_1,\cdots,r_s}(i+1) = \frac{1}{n-i}S_{j,r_1,\cdots,r_s}(i)+\frac{1}{(n-i)(i+1)^j}S_{r_1,\cdots,r_s}(i+1)\tag{21}$$

Partial fractioning of the last term will leave something simpler. Similarly there is:

$$\frac{1}{n-i}S_{j,r_1,\cdots,r_s}(i-1) = \frac{1}{n-i}S_{j,r_1,\cdots,r_s}(i)-\frac{1}{(n-i)(i-1)^j}S_{r_1,\cdots,r_s}(i-1)\tag{22}$$

For two S-functions one can write:

$$\begin{aligned}S_{j,r_1,\cdots,r_s}(n-i)S_{k,p_1,\cdots,p_s}(i+1) &= S_{j,r_1,\cdots,r_s}(n-i)S_{k,p_1,\cdots,p_s}(i)\\ &\quad +\frac{1}{(i+1)^k}S_{j,r_1,\cdots,r_s}(n-i)S_{p_1,\cdots,p_s}(i+1)\\ &= S_{j,r_1,\cdots,r_s}(n-i)S_{k,p_1,\cdots,p_s}(i)\\ &\quad +\frac{1}{(i+1)^k}S_{j,r_1,\cdots,r_s}(n-i-1)S_{p_1,\cdots,p_s}(i+1)\\ &\quad +\frac{1}{(i+1)^k(n-i)^j}S_{r_1,\cdots,r_s}(n-i)S_{p_1,\cdots,p_s}(i+1)\end{aligned}\tag{23}$$

Again partial fractioning of the last term leads to a simpler object. One can derive equivalent relations for combinations involving factorials. In this case also pairs of factorials can be dealt with:

$$\begin{aligned}\frac{1}{(n-i)!\ (i+1)!} &= \frac{1}{(n-i-1)!\ i!}\frac{1}{n+1}\left(\frac{1}{n-i}+\frac{1}{i+1}\right)\\ &= \frac{1}{n+1}\left(\frac{1}{(n-i)!\ i!}+\frac{1}{(n-i-1)!\ (i+1)!}\right)\end{aligned}\tag{24}$$

All the above relations can be combined into one recursion that leaves all S-functions, all denominators and at least one factorial properly synchronized. Additionally one has a proper adjustment to the boundaries of the summation, and therefore the factorials can often be combined into binomial coefficients.

4 Mellin Transforms

The Mellin operator M is defined by

$$M(f(x)) = \int_0^1 dx\ x^m f(x) \tag{25}$$

and the operator M^+ by

$$M^+(f(x)) = \int_0^1 dx\ x^m \frac{f(x)}{(1-x)_+} \tag{26}$$

with

$$\int_0^1 dx \frac{f(x)}{(1-x)_+} = \int_0^1 dx \frac{f(x) - f(1)}{1-x} \tag{27}$$

when $f(1)$ is finite. When there is a power of $\ln(1-x)$ present it becomes

$$M^+((\ln(1-x))^k f(x)) = \int_0^1 dx\ x^m \frac{(\ln(1-x))^k f(x)}{(1-x)_+} \tag{28}$$

$$= \int_0^1 dx(f(x) - f(1)) \frac{(\ln(1-x))^k}{1-x} \tag{29}$$

These are the traditional operations. In the literature one often defines the transform shifted over one as in

$$M(f(x)) = \int_0^1 dx\ x^{N-1} f(x) \tag{30}$$

In the context of this paper the notation will be the one of equation (25). The 'Mellin parameter' is given in that case in lower case variables. Hence the translation to the shifted notation should be of the nature $n \to N-1$.

For Mellin transforms of formulas resulting from Feynman diagrams one has to consider the transforms of functions that are combinations of $1/(1-x)_+$, $1/(1+x)$, $\ln(x)$, $\ln(1+x)$, $\ln(1-x)$, powers of these logarithms, and various polylogarithms of which the arguments are rational functions of x. Powers of x just change the moment of the function. Hence they do not have to be considered. Additionally one can always assume that either $1/(1-x)_+$ or $1/(1+x)$ is present, because the functions without such a term can be written as two functions in the class that is being considered:

$$1 = \frac{1}{1+x} + \frac{x}{1+x} \tag{31}$$

The algorithm that obtains the Mellin transform of any combination of such functions is rather direct. Consider the following steps:

1. If there is a power of $1/(1-x)$ or $1/(1+x)$, replace it by a sum according to the formulas

$$\frac{x^m}{1-x} = \sum_{i=m}^{\infty} x^i \tag{32}$$

$$\frac{x^m}{1+x} = (-1)^m \sum_{i=m}^{\infty} (-1)^i x^i \tag{33}$$

2. If the function to be transformed contains powers of $\ln(1-x)$, split it into its powers of $\ln(1-x)$ and $F(x)$ which represents the rest and has a finite value at $x = 1$. Then one writes

$$\int_0^1 dx\ x^m \ln^p(1-x)\ F(x) = \int_0^1 dx\ x^m \ln^p(1-x)\ (F(x) - F(1)) + F(1) \int_0^1 dx\ x^m \ln^p(1-x) \tag{34}$$

3. The Mellin transform of just a power of $\ln(1-x)$ can be replaced immediately using the formula
$$\int_0^1 dx\ x^m \ln^p(1-x) \quad = \quad \frac{(-1)^p p!}{m+1} S_{1,\cdots,1}(m+1) \tag{35}$$
in which the S-function has p indices that are all 1. This avoids divergence problems during the next step. Similarly one can apply:
$$\int_0^1 dx\ x^m \ln^p(x) = \frac{(-1)^p p!}{(m+1)^{p+1}} \tag{36}$$
when there is only a power of $\ln(x)$ left, but this step is not essential; it only makes the algorithm a bit faster. Due to the powers of x there will be no divergence problems near $x = 0$.

4. Do a partial integration on the powers of x. Because of the second step, the values at $x = 0$ and $x = 1$ never present any problems.

5. If there is only a power of x left one can integrate and the integration phase is finished. Otherwise one should repeat the previous steps until all functions have been broken down. Note that for this to work all functions have to break down properly. Hence one cannot use fractional powers of the functions involved.

6. At this point the terms may contain nested sums, either to a finite upper limit or to infinity. These sums do not present any complications once products of two S-functions with identical arguments can be combined into elements of the natural basis (see appendix A).

The main complication in the above algorithm is the treatment of the infinities that may arise in the summations. Many of the terms develop a divergence. These are all of a rather soft nature and hence their regularization is relatively easy. All divergences in the sums are of a logarithmic nature and hence, if one considers the sum to go to a rather large integer L, the divergent sums behave like powers of $\ln L$ up to terms of order $1/L$[1]. Because all transforms should be finite the terms in $\ln L$ should cancel. After that one can safely take the limit $L \to \infty$. Taking this all in consideration, all sums that contain a divergence can be rewritten into powers of one single basic divergent sum $(S_1(\infty))$ and finite terms. After that there are no more problems of this nature.

The result of the above algorithm is an expression with many harmonic series of which the argument is a function of m and others of which the argument is infinity. These last sums are treated in the next section.

5 Values at Infinity

In the previous section the results of the Mellin transforms were harmonic series in the Mellin parameter m and harmonic series at infinity. In order to solve the problem completely one has to find the values for these series at infinity. After all they represent finite numbers and the number of series is much larger than the number of transcendental numbers that occur once they are evaluated. The sums to be considered are related to the Euler-Zagier sums [9] [10] [11] which are defined as
$$\zeta(s_1,\ldots,s_k;\sigma_1,\ldots,\sigma_k) = \sum_{n_j > n_{j+1} > 0} \prod_{j=1}^{k} \frac{\sigma_j^{n_j}}{n_j^{s_j}}\ . \tag{37}$$

[1]In principle there is also an Euler constant, but when the logarithms cancel, also the Euler constants cancel and hence they are not considered here

These sums are however not identical to the S-functions at infinity because for them the sum is

$$S_{s_1,\ldots,s_k}(\infty) = \sum_{n_j \geq n_{j+1} \geq 1} \prod_{j=1}^{k} \frac{[(-1)^{n_j}]_{s_j<0}}{n_j^{|s_j|}}. \tag{38}$$

The notation $[\ \ ]_{s_1<0}$ indicates that this part is present only when $s_1 < 0$. Here a method is presented to evaluate these sums that is completely different from the one in reference [11].

The first step in the evaluation of the sums is to express the sums as much as possible in terms of products of harmonic series with a lower weight. This can be done up to a point. One will always need a number of series with the weight one is considering. This step is basically the inverse of the algorithm of appendix A. It is harder to be implemented in a deterministic way, because the choice of the basis is not unique. But this can be solved in a different way as will be seen below.

Next there are two types of extra identities one can consider. The first set comes from looking at the series with only positive indices and applying the doubling formula (6) to it. For all the series that are finite it makes no difference whether the argument is infinity or two times infinity. If the selected basis is such that all divergences are powers of $S_1(\infty)$ one only has to make the extra adjustment $S_1(2\infty) \to S_1(\infty) + \ln(2)$. This gives a number of extra equations that correspond to new relations between the series. Unfortunately this does not give enough relations, but some are interesting in their own right. For instance

$$S_m(\infty) \quad = \quad 2^{m-1}(S_m(2\infty) + S_{-m}(2\infty)) \tag{39}$$

gives immediately the well known relations

$$\begin{aligned} S_{-m}(\infty) \quad &= \quad -(1 - 2^{1-m})S_m(\infty) \qquad\qquad m > 1 && (40)\\ S_{-1}(\infty) \quad &= \quad -\ln(2) && (41) \end{aligned}$$

The more powerful consideration however is the following: Suppose one is summing over a square grid of size $n \times n$. Under what conditions is the sum over the upper right diagonal half of the square $(i_1 + i_2 > n)$ zero in the limit $n \to \infty$? If this sum is zero, the product over two individual sums can be replaced by a sum over the lower left diagonal triangle $(i_1 + i_2 \leq n)$. This leads to the following theorem:

Theorem: When not both $m_1 = 1$ and $k_1 = 1$ the following identity holds:

$$S_{m_1,\cdots,m_p}(\infty)S_{k_1,\cdots,k_q}(\infty) \quad = \quad \lim_{n\to\infty} \sum_{i=1}^{n} S_{m_1,\cdots,m_p}(n-i)S_{k_2,\cdots,k_q}(i)\frac{[(-1)^i]_{k_1<0}}{i^{|k_1|}} \tag{42}$$

The proof is rather trivial, considering that all m_i and k_i are integers and that alternate series with $(-1)^i$ actually converge one power of i better than they seem to at first sight. This can be seen when the terms are grouped in pairs. The sums can be estimated by integrals and the numerators can only give powers of logarithms. Hence the presence of at least three powers of denominators (excluding $m_1 = k_1 = 1$) will make the limit go to zero.

The sum can be readily worked out with the algorithm described in appendix C.

Assume that all sums up to weight n have been determined. The complete algorithm for weight $n+1$ is now:

1. Construct all pairs of S-functions for which the sum of the two weights is $n+1$.

2. Each pair is used to construct two equations (unless both S-functions have their first index equal to one in which case the second equation that would have been based on the above

theorem is not made). The first equation is made by taking $S^{(1)}S^{(2)} - S^{(1)}S^{(2)}$ and applying the routine (see appendix A) that converts the S-functions to the basis to the first pair. These are the 'shuffle algebra' relations. The second set of equations is created by taking $S^{(1)}S^{(2)} - S^{(1)}S^{(2)}$ and then applying the formula of the theorem to the first pair. After this the routine of appendix C is applied.

3. Substitute the values for the lower S-functions.

4. Eliminate now the 'unknown' S-functions of weight $n+1$ as much as possible as if one is solving a linear set of equations (which is what it is). Apply the same set of substitutions that will eliminate the equations to the series that need to be evaluated.

5. Inspect the result and see which sums should be considered as new independent variables because they were not eliminated. If one insists on a given sum to be among the variable(s) not to be eliminated one can substitute it by a different variable before the elimination procedure.

It is not so difficult to construct a program in the language of FORM that can execute this procedure all the way to S-functions of weight 7. Such a program takes just a few hours (< 6 without special optimizations) on a Pentium-II-300 processor. When a series diverges one uses the basic divergence $S_1(\infty)$ as if it were a regular variable. This presents no problems.

The variables that one needs at the different weights are: $S_1(\infty)$, $\ln(2)$, ζ_2, ζ_3, $\mathrm{Li}_4(\frac{1}{2})$, ζ_5, $\mathrm{Li}_5(\frac{1}{2})$, $\mathrm{Li}_6(\frac{1}{2})$, $S_{-5,-1}(\infty)$, ζ_7, $\mathrm{Li}_7(\frac{1}{2})$, $S_{-5,1,1}(\infty)$, $S_{5,-1,-1}(\infty)$. The choice of the S-functions that remain is not unique. Here the selection is such that they contain as few indices as possible and are as convergent as possible. Numerical values for these quantities can be obtained by standard techniques.

$$
\begin{aligned}
\mathrm{Li}_4(1/2) &= 0.51747906167389938633 \\
\mathrm{Li}_5(1/2) &= 0.50840057924226870746 \\
\mathrm{Li}_6(1/2) &= 0.50409539780398855069 \\
\mathrm{Li}_7(1/2) &= 0.50201456332470849457 \\
S_{-5,-1}(\infty) &= 0.98744142640329971377 \\
-S_{-5,1,1}(\infty) &= 0.95296007575629860341 \\
S_{5,-1,-1}(\infty) &= 1.02912126296432453422
\end{aligned}
\tag{43}
$$

It should be noted however that according to the work by Broadhurst and Kreimer [12] most of these constants should not appear in the computation of massless Feynman diagrams. The first non-zeta constant should be $S_{5,3}(\infty)$ which is an object of weight 8. This indicates that in x-space the functions can only occur in such combinations that these constants cancel in Mellin space. Hence one may not need to know their values for many applications. In the case of massive Feynman diagrams the situation is different. The constant $\mathrm{Li}_4(1/2)$ does occur in the three loop corrections to the $g-2$ of the electron [13].

The results of the runs up to weight 7 have been tabulated and put in the FORM program. The main problem in making the tables is that the objects with identical weights may have different numbers of indices. Hence the notation of indices that are either -1, 1 or 0 of equation (8) is used for the tables. The conversion to and from this notation is rather simple.

6 Inverse Mellin Transforms

If one can obtain a result in Mellin space (as a function of n) in principle it is possible to convert to the function in x-space. This is however a rather complicated operation. There exists some literature about it [2] [7] but it remains rather difficult. Also considering it as some type of Laplace transform does not give much relief [8]. In many cases one can employ a different strategy. Given a result in Mellin space with a set of series, one can try to find a set of functions in x-space for which the Mellin transforms span the space of the functions in Mellin space. After that one only has to solve a set of linear equations to make the inverse transform. In the case of two loop moments of structure functions in deep inelastic scattering, the results in Mellin space are just S-functions of weight 4. Because the whole space of such S-functions is 54 dimensional (a basis has 54 elements) one has to find 54 functions in x-space that map into the Mellin space in a linearly independent way. This does not present too many problems. One should of course note that this method depends on having routines to do the Mellin transforms automatically.

For higher weights it may not be so easy to find a complete set of functions in x-space. This can be illustrated by a simple calculation. To obtain a complete set of functions in x-space for which the Mellin transforms cover the natural basis of weight w one needs $2 \times 3^{w-1}$ functions in x-space. Because this number can be divided by two (the relevant functions are of the types $f(x)/(1 \pm x)$) only 3^{w-1} functions have to be considered. A number of these can be constructed by taking products of functions that contribute to lower weights. That leaves a number of functions that are new at the given weight. This number increases rapidly with the weight. They are $3, 8, 18, 48, 116$ for the weights $3, 4, 5, 6, 7$ respectively. Hence one has to come up with a rather large number of new functions when the weight becomes large. Fortunately there is a method that will work provided only a numerical answer is needed for any value of x.

Assume that for a given weight w all necessary functions in x-space are known. Assume also that the Mellin transform of some F is given by

$$\int_0^1 dx\ x^n F(x) \quad = \quad \frac{S_{\overrightarrow{m}}(n+1)}{(n+1)^p} \tag{44}$$

in which $\overrightarrow{m}$ represents any allowable series of the type $m_1, \cdots, m_q$ and $p > 0$. For this function F one has

$$\int_0^1 dx\ x^n \frac{F(x)}{1+x} \quad = \quad (-1)^n S_{-p,\overrightarrow{m}}(n) - (-1)^n S_{-p,\overrightarrow{m}}(\infty) \tag{45}$$

$$\int_0^1 dx \frac{x^n F(x)}{(1-x)_+} \quad = \quad S_{p,\overrightarrow{m}}(\infty) - S_{p,\overrightarrow{m}}(n) - S_1(\infty)F(1) \tag{46}$$

In the second expression one can see that $F(1)$ will be nonzero when $p = 1$ and zero otherwise. This is needed to keep the expression finite. It is assumed here that $F(x)$ does not contain a factor $\ln(1-x)$ or that if it does the other components of F still make that $F(1) = 0$. If this is not the case there will be more complicated sums of the type of appendix D and the right hand side will have more terms to cancel the divergences that are due to $S_{p,\overrightarrow{m}}(\infty)$ having more than one power of $S_1(\infty)$. Rather than using the sums of appendix D one can also use the algorithms of section 4 to break down the function F completely.

Considering that a knowledge of all odd or all even moments is sufficient to reconstruct F the presence of $(-1)^n$ should not be a problem in the end. It does not lead to a doubling of the necessary functions –even moments in terms of N correspond to odd moments in terms of n–. One should also observe now that the functions $F(x)/(1+x)$ and $F(x)/(1-x)$ are related to the inverse Mellin transforms of $S_{-p,\overrightarrow{m}}(n)$ and $S_{p,\overrightarrow{m}}(n)$ respectively. Assume now that the $S_{p,\overrightarrow{m}}(n)$ are of weight w.

How does one construct the inverse Mellin transforms of functions of weight $w+1$? For this one should have a look at the functions

$$
\begin{aligned}
F^{+}(x) &= \int_0^x dx \frac{F(x)}{1+x} && (47)\\
F^{-}(x) &= \int_0^x dx \frac{F(x)}{1-x} && (48)\\
F^{0}(x) &= \int_x^1 dx \frac{F(x)}{x} && (49)
\end{aligned}
$$

For these functions one can derive readily by means of partial integration

$$
\begin{aligned}
\int_0^1 dx\ x^n F^{+}(x) &= -\frac{(-1)^{n+1}}{n+1} S_{-p,\overrightarrow{m}}(n+1) + \frac{1}{n+1}((-1)^{n+1}-1)S_{-p,\overrightarrow{m}}(\infty) && (50)\\
\int_0^1 dx\ x^n F^{-}(x) &= \frac{1}{n+1} S_{p,\overrightarrow{m}}(n+1) && (51)\\
\int_0^1 dx\ x^n F^{0}(x) &= -\frac{1}{(n+1)^{p+1}} S_{\overrightarrow{m}}(n+1) && (52)
\end{aligned}
$$

With the aid of equations (45) and (46) one derives now the relations

$$
\begin{aligned}
\int_0^1 dx\ x^n \frac{F^{+}(x)}{1+x} &= -(-1)^n S_{1,-p,\overrightarrow{m}}(n) + (-1)^n (S_{1,-p,\overrightarrow{m}}(\infty) - S_1(\infty) S_{-p,\overrightarrow{m}}(\infty))\\
&\quad +(-1)^n S_{-p,\overrightarrow{m}}(\infty)(S_1(n) - S_{-1}(n) + S_{-1}(\infty)) && (53)\\
\int_0^1 dx\ x^n \frac{F^{-}(x)}{1+x} &= (-1)^n (S_{-1,p,\overrightarrow{m}}(n) - S_{-1,p,\overrightarrow{m}}(\infty)) && (54)\\
\int_0^1 dx\ x^n \frac{F^{0}(x)}{1+x} &= (-1)^n (-S_{-(p+1),\overrightarrow{m}}(n) + S_{-(p+1),\overrightarrow{m}}(\infty)) && (55)\\
\int_0^1 dx \frac{x^n F^{+}(x)}{(1-x)_+} &= S_{-1,-p,\overrightarrow{m}}(n) - S_{-1,-p,\overrightarrow{m}}(\infty)\\
&\quad +S_{-p,\overrightarrow{m}}(\infty)(S_{-1}(\infty) - S_{-1}(n) + S_1(n)) && (56)\\
\int_0^1 dx \frac{x^n F^{-}(x)}{(1-x)_+} &= -S_{1,p,\overrightarrow{m}}(n) + S_{1,p,\overrightarrow{m}}(\infty) - S_1(\infty) S_{p,\overrightarrow{m}}(\infty) && (57)\\
\int_0^1 dx \frac{x^n F^{0}(x)}{(1-x)_+} &= S_{(p+1),\overrightarrow{m}}(n) - S_{(p+1),\overrightarrow{m}}(\infty) && (58)
\end{aligned}
$$

In these expressions is assumed that $F(x)$ contains no factors $\ln(1-x)$. In that case it is not difficult to see that all divergences cancel. When there are factors $\ln(1-x)$ the expressions become a bit more complicated in the constant terms in order to obtain a complete cancellation of the divergences. The first terms of the right hand side expressions form indeed a complete set of S-functions of weight $w+1$ when all possible values of p and all possible S-functions in equation (44) are considered. Because all other terms in the right hand side expressions are of a lower weight in terms of the argument n, their inverse Mellin transforms are supposed to be known and hence all inverse Mellin transforms of weight $w+1$ can be constructed. If the integrals in the definitions of F^{+}, F^{-} and F^{0} cannot be solved analytically, one can still obtain their values numerically by standard integration techniques. If one has to go more than one weight beyond what is analytically possible, one obtains multiple integrals. Many of these can of course be simplified by partial integrations as can be seen in the following formula:

$$
F^{++}(x) = \int_0^x \frac{dx}{1+x} \int_0^x \frac{dx}{1+x} F(x) \qquad (59)
$$

$$= \ln(1+x)\int_0^x \frac{dx}{1+x}F(x) - \int_0^x \frac{\ln(1+x)\ F(x)}{1+x}dx \tag{60}$$

At this point it seems best to give some examples. First look at the constant function in Mellin space. It is the only function with weight zero and its inverse Mellin transform is $\delta(1-x)$. Here $\delta(x)$ is the Dirac delta function. Hence the inverse Mellin transforms for functions with weight one are:

$$(-1)^n S_{-1}(n) \rightarrow \frac{1}{1+x} + (-1)^n \ln(2)\ \delta(1-x) \tag{61}$$

$$S_1(n) \rightarrow -\frac{1}{1-x} \tag{62}$$

The factor $(-1)^n$ in the right hand side indicates that the reconstruction from the even moments different from the reconstruction from the odd moments. This means that if the moments are obtained for even values of N (which means odd values for n) one should treat the terms in $S_{\overrightarrow{m}}(n)$ differently from the terms in $S_{\overrightarrow{m}}(n+1)$.

Next are the functions with weight 2. The only function with weight one that can occur in equation (44) is $1/(n+1)$ and its inverse Mellin transform is given by $F(x) = 1$. From this one can construct $F^+(x) = \ln(1+x)$, $F^-(x) = -\ln(1-x)$ and $F^0(x) = \ln(x)$. One can now work out the equations (53 - 58) to obtain the inverse Mellin transforms for the weight two functions.

For the weight three functions one obtains dilogarithms with the arguments $x, -x$ and $(1+x)/2$ as new objects. For the weight four functions the functions $F^{\pm}(x)$ and $F^0(x)$ can have trilogs with the arguments $x, -x$, $(1+x)/2$, $1/(1+x)$, $1-x$, $2x/(1+x)$, $(1-x)/(1+x)$ and $-(1-x)/(1+x)$. Of course one may choose a different representation in which the function $S_{1,2}(x)$ plays a rôle (see references [14] and [15]).

There is one more important observation to be made. The expressions (53-58) have just a single S-function of weight $w+1$ in the right hand side. This means that one can obtain the inverse Mellin transforms of the various S-functions without having to solve sets of equations. One only has to move terms from the right hand side and put their inverse Mellin transform (which is much simpler) into the various F-functions. This can be done systematically and it can be checked by the Mellin transformation program. The approach of looking for which functions can occur and then making their Mellin transform and inverting the set of equations would lead to very complicated sets of equations when the weights become large. Hence the interesting functions are more or less the ones that have been built up from the original weight one functions by composing higher and higher integrals like $F^{+-0++0}(x)$ etc. without writing the result in terms of individual polylogarithms.

7 Some applications

The values at infinity of the previous section have some rather relevant applications for certain classes of integrals. This can best be illustrated with some examples. The following integral would under normal circumstances be rather difficult, but with all the above tools it becomes rather trivial:

$$\int_0^1 dx \frac{\ln(x)\ \ln^2(1-x)\ \ln(1+x)}{x} = -\sum_{i=0}^{\infty} \frac{1}{i+1}\int_0^1 dx\ x^i\ \ln(x)\ \ln(1-x)\ \ln(1+x) \tag{63}$$

The integral is just one of the Mellin transformations, and hence the program will handle it. The sum is of the same type as all other sums in the Mellin transformation and hence will be done also by the program. In the end the answer is expressed in terms of S-functions at infinity which are maximally of weight 5 and hence they can be substituted from the tables. The final result is:

$$\int_0^1 dx \frac{\ln(x)\ \ln^2(1-x)\ \ln(1+x)}{x} = -\frac{3}{8}\zeta_2\zeta_3 - \frac{2}{3}\zeta_2\ln^3(2) + \frac{7}{4}\zeta_3\ln^2(2) - \frac{7}{2}\zeta_5 + 4\ln(2)\ \mathrm{Li}_4(1/2) + \frac{2}{15}\ln^5(2) + 4\ \mathrm{Li}_5\ (1/2) \tag{64}$$

Similarly one obtains

$$\int_0^1 dx \frac{\ln(x)\ \ln^2(1-x)\ \ln^2(1+x)}{x} = -\frac{1}{2}\zeta_2\ln^4(2) - \frac{129}{140}\zeta_2^3 + \frac{7}{6}\zeta_3\ln^3(2) - \frac{37}{16}\zeta_3^2 - \frac{31}{8}\zeta_5\ln(2) + 8\ln(2)\ \mathrm{Li}_5(1/2) + 4\ln^2(2)\ \mathrm{Li}_4(1/2) + \frac{1}{9}\ln^6(2) + 8\ \mathrm{Li}_6(1/2) + 2\ S_{-5,-1}(\infty) \tag{65}$$

and the even more difficult integral

$$\int_0^1 dx \frac{\ln(1-x)\mathrm{Li}_2(\frac{1+x}{2})\mathrm{Li}_3(\frac{1-x}{1+x})}{1+x} = -\frac{7}{4}\zeta_2\zeta_3\ln^2(2) - \frac{5673}{448}\zeta_2\zeta_5 - 5\zeta_2\ln(2)\ \mathrm{Li}_4(1/2) - \frac{17}{120}\zeta_2\ln^5(2) - 5\zeta_2\mathrm{Li}_5(1/2) + \frac{1517}{1120}\zeta_2^2\zeta_3 + \frac{5}{6}\zeta_2^2\ln^3(2) - \frac{1}{84}\zeta_2^3\ln(2) - \frac{7}{96}\zeta_3\ln^4(2) - \frac{3}{4}\zeta_3\mathrm{Li}_4(1/2) - \frac{1563}{448}\zeta_3^2\ln(2) - \frac{93}{32}\zeta_5\ln^2(2) + \frac{74415}{1792}\zeta_7 - 18\ln(2)\ \mathrm{Li}_6(1/2) - \frac{43}{14}\ln(2)\ S_{-5,-1}(\infty) - 6\ln^2(2)\ \mathrm{Li}_5(1/2) - \ln^3(2)\ \mathrm{Li}_4(1/2) - \frac{1}{84}\ln^7(2) - 24\ \mathrm{Li}_7(1/2) - \frac{45}{7}S_{-5,1,1}(\infty) + \frac{32}{7}S_{5,-1,-1}(\infty) \tag{66}$$

As one can see, this technique allows the evaluation of whole classes of integrals that go considerably beyond the integrals in ref [14].

Another application of the techniques of the previous sections concerns the evaluation of certain classes of Feynman diagrams. When one tries to evaluate moments of structure functions in perturbative QCD one has Feynman diagrams which contain the momenta P and Q. Assuming that the partons are massless one has that $P^2 = 0$ and because all dimensions are pulled out of the integral in the form of powers of Q^2, there is only a single dimensionless kinematic variable left which is $x = 2P{\cdot}Q/Q^2$. The power series expansion in terms of P before integration corresponds to the expansion in terms of Mellin moments of the complete function after integration. The complete functions have been calculated for the two loop level [15] but for the three loop level the calculation could only be done for a small number of fixed moments $2, 4, 6, 8$ and in one case also 10 [16]. To evaluate all these moments requires that the expansion in P should be in terms of a symbolic power N. This will introduce sums and these sums will be expressed in terms of harmonic series. After all integrals have been done all attention has to be focussed on the summations and it is actually for this purpose that the program SUMMER has been developed. By now a general two loop program has been constructed [17] and studies are on their way to create a three loop program. It should be noted that in the two loop program no series at infinity can occur. This puts a restriction on the functions that can occur in x-space. They have to appear in such linear combinations that all the constants (with the exception of ζ_3 which comes from expansions of the Γ-function) should cancel in the Mellin transform.

8 Conclusions

The algorithms presented in this paper provide a base for working with the sums that can occur in many types of calculations, one of which is the evaluation of Feynman diagrams in deep inelastic scattering. Additionally they allow the analytic evaluation of whole classes of integrals. The problem of the Mellin transforms of whole categories of functions has been solved, and a numerical solution for inverse Mellin transforms has been given. Most of the algorithms and tables have been programmed in the language of FORM version 3 and are available from the homepage of the author (http://norma.nikhef.nl/∼t68/summer).

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A Conversion to the Basis

To convert products of S-functions with an identical last argument to the basis of single higher S-functions one can use a recursion. If one starts with the functions $S^{(1)}$ and $S^{(2)}$ and accumulates the results into the function $S^{(3)}$ the recursion reads:

$$\begin{aligned} S^{(1)}_{m_1j_1\cdots j_r}(n)S^{(2)}_{m_2p_1\cdots p_s}(n)S^{(3)}_{q_1\cdots q_t}(n) \;\rightarrow\; & S^{(1)}_{m_1j_1\cdots j_r}(n)S^{(2)}_{p_1\cdots p_s}(n)S^{(3)}_{q_1\cdots q_tm_2}(n) \\ & +S^{(1)}_{j_1\cdots j_r}(n)S^{(2)}_{m_2p_1\cdots p_s}(n)S^{(3)}_{q_1\cdots q_tm_1}(n) \\ & -S^{(1)}_{j_1\cdots j_r}(n)S^{(2)}_{p_1\cdots p_s}(n)S^{(3)}_{q_1\cdots q_t(m_1\&m_2)}(n) \end{aligned} \tag{67}$$

The recursion starts with $S^{(3)}(n)=1$ and the recursion terminates when either $S^{(1)}(n)$ or $S^{(2)}(n)$ has no more indices and hence can be replaced by 1 after which

$$S^{(a)}_{j_1\cdots j_r}(n)S^{(3)}_{q_1\cdots q_t}(n) \;\rightarrow\; S_{q_1\cdots q_tj_1\cdots j_r}(n) \tag{68}$$

with $a=1,2$. Because this is a direct construction of the result, it is rather fast. It can be implemented in the language of FORM (version 3 or higher) very efficiently:

```
repeat;
  id,once,S(R(?a),n?)*S(R(?b),n?) = SS(R(?a),R,R(?b),n);
  repeat id SS(R(m1?,?a),R(?b),R(m2?,?c),n?) =
              +SS(R(m1,?a),R(?b,m2),R(?c),n)
              +SS(R(?a),R(?b,m1),R(m2,?c),n)
              -SS(R(?a),R(?b,m1*sig_(m2)+m2*sig_(m1)),R(?c),n);
  id,SS(R(?a),R(?b),R(?c),n?) = S(R(?b,?a,?c),n);
endrepeat;
```

Note that the function SS carries the indices of $S^{(1)}$, $S^{(3)}$ and $S^{(2)}$ in this order. The function sig_ returns the sign of its argument. Hence the expression that uses this function is one way of writing the pseudo addition &.

The above code has been made into a FORM procedure. A rather nontrivial test program could be:

```
#-
#include nndecl.h
.global
```

```
L F = S(R(1,1,1,1,1),n)*S(R(-1,-1,-1,-1,-1),n);
#call basis(S);
.end
```

It gives the result

```
Time =        0.64 sec    Generated terms =      1683
                 F        Terms in output =      1683
                          Bytes used      =     85104
```

The run was made on a Pentium Pro 200 chip running the NeXTstep operating system. As one can see, these expressions can become rather complicated. On the other hand, weight 10 functions are of course not trivial. It should be noted that it is relatively easy to test routines like the one above. One can try them out for any functions and any values of the argument and evaluate the corresponding harmonic series into a rational number and see that they are identical.

B Conjugations

For the conjugations one should consider only S-functions with positive indices. The conjugation is defined with the sum

$$(f(n))^C = -\sum_{i=1}^{n}(-1)^i \binom{n}{i} f(i) \tag{69}$$

That this is a conjugation can be shown easily by applying it twice. This gives the original function. For the function f one can use S-functions or the combination of an S-function and a negative power of the argument of the S-function as in $S_{j_1\cdots j_r}(n)/n^k$. For these functions one has:
Theorem: The conjugate function of an element of the natural basis with only positive indices is a single S-function of a lower weight with only positive indices, combined with enough negative powers of its argument to give the complete term the same extended weight as the original function.
Proof: First look at the weights one and two:

$$\begin{aligned}
(S_1(n))^C &= 1/n && (70)\\
(S_2(n))^C &= S_1(n)/n && (71)\\
(S_{1,1}(n))^C &= 1/n^2 && (72)
\end{aligned}$$

They clearly fulfill the theorem. Then write

$$(S_{mj_1\cdots j_r}(n))^C = \frac{1}{n}(S_{j_1\cdots j_r}(n)/n^{m-1})^C \tag{73}$$

This identity can be obtained by writing the outermost sum and then exchanging it with the sum of the conjugation. Assume now that the theorem holds for all functions with a lower weight. There are two cases: $m = 1$ and $m > 1$. When $m = 1$ the problem has been reduced to the same problem of finding the conjugate but now for a function with a lower extended weight. Hence, if the theorem holds for all simpler functions it holds also at the current weight. For $m > 1$ the conjugate of $S_{j_1\cdots j_r}(n)/n^{m-1}$ must be a single harmonic function of weight $m-1$. This can be seen when one realizes that for each extended weight there are as many functions with their 'proper' weight equal to this extended weight as with their 'proper' weight less than the extended weight. Hence the function must have a conjugate that is a single S-function. Together with the fact that two conjugations give the original function, and the fact that all S-functions of a given weight are linearly independent this completes the proof of the theorem.

Next is the derivation of an algorithm to find the conjugate of $S_{j_1\cdots j_r}(n)/n^{m-1}$. One way would be to successively build up the algorithm by first deriving all conjugates up to a given weight. After that one can obtain the needed conjugates by reading the formulae backwards. This is not very elegant. For a more direct way one can define the concept of the associate function.

$$S^A_{j_1\cdots j_r}(n) = \sum_{i=1}^{n}(S_{j_1\cdots j_r}(i))^C \tag{74}$$

Note that because $X = S_{j_1\cdots j_r}$ is an element of the basis, $(X(i))^C$ contains powers of $1/i$ and the sum gives again a single harmonic function of the same weight as X. It is rather easy to prove that $(X^A)^A = X$. The task of finding the conjugate can now be reduced to the task of finding the associate function. If this associate function can be written as $S_{mj_1\cdots j_r}(n)$ the conjugate will be $S_{j_1\cdots j_r}(n)/n^m$. Similarly a function in combination with negative powers of n can be rewritten as a sum $(S_{j_1\cdots j_r}(n)/n^m \to S_{mj_1\cdots j_r}(n))$, and then the associate function of this function will be the needed conjugate function.

The associate function can be found by construction. Assume that $(S_{j_1\cdots j_r}(n))^A = S_{mp_1\cdots p_s}(n)$. Then

$$\begin{aligned}
(S_{1j_1\cdots j_r}(n))^A &= \sum_{i=1}^{n}(S_{1j_1\cdots j_r}(i))^C \\
&= \sum_{i=1}^{n}\frac{1}{i}(S_{j_1\cdots j_r}(i))^C \\
&= \sum_{i=1}^{n}\frac{1}{i}\frac{S_{p_1\cdots p_s}(i)}{i^m} \\
&= S_{(m+1)p_1\cdots p_s}(n)
\end{aligned} \tag{75}$$

and similarly for $k > 1$:

$$\begin{aligned}
(S_{kj_1\cdots j_r}(n))^A &= \sum_{i=1}^{n}(S_{kj_1\cdots j_r}(i))^C \\
&= \sum_{i=1}^{n}\frac{1}{i}(\frac{S_{j_1\cdots j_r}(n)(i)}{i^{k-1}})^C \\
&= \sum_{i=1}^{n}\frac{1}{i}(S_{(k-1)j_1\cdots j_r}(i))^A \\
&= S_{1q_1\cdots q_t}(n)
\end{aligned} \tag{76}$$

with $(S_{(k-1)j_1\cdots j_r}(n))^A = S_{q_1\cdots q_t}(n)$. Considering that $(S_1(n))^A = S_1(n)$ associate functions to any weight can now be constructed. This algorithm is also easy to implement in a program like FORM.

C Sums involving $n - i$

In this appendix sums of the type

$$\sum_{i=1}^{n-1}\frac{S_{p_1\cdots p_s}(n-i)S_{q_1\cdots q_t}(i)}{i^k} \tag{77}$$

will be considered. It is impossible to combine the sums to a single basis element. Hence a different method is called for. Assume first that $k > 0$ and $m > 0$ (below). Writing out the outermost sum of the S-function with the argument $n-i$ leads to

$$\begin{aligned}
\sum_{i=1}^{n-1} \frac{S_{mp_1\cdots p_s}(n-i)S_{q_1\cdots q_t}(i)}{i^k} &= \sum_{i=1}^{n}\sum_{j=1}^{n-i} \frac{S_{p_1\cdots p_s}(j)}{j^m}\frac{S_{q_1\cdots q_t}(i)}{i^k} \\
&= \sum_{i=1}^{n}\sum_{j=i+1}^{n} \frac{S_{p_1\cdots p_s}(j-i)}{(j-i)^m}\frac{S_{q_1\cdots q_t}(i)}{i^k} \\
&= \sum_{j=1}^{n}\sum_{i=1}^{j-1} \frac{S_{p_1\cdots p_s}(j-i)}{(j-i)^m}\frac{S_{q_1\cdots q_t}(i)}{i^k} \\
&= \sum_{i=1}^{n}\sum_{j=1}^{i-1} S_{p_1\cdots p_s}(i-j)S_{q_1\cdots q_t}(j)\frac{1}{(i-j)^m j^k} \qquad (78)
\end{aligned}$$

Partial fractioning of the denominators gives sums in which the denominator is a power $k' \leq k$ of j and sums in which the denominator is a power $m' \leq m$ of $i-j$. These last sums can be done immediately by reverting the direction of summation. Hence:

$$\begin{aligned}
\sum_{i=1}^{n-1} \frac{S_{mp_1\cdots p_s}(n-i)S_{q_1\cdots q_t}(i)}{i^k} &= \sum_{a=1}^{k}\binom{k+m-1-a}{m-1}\sum_{i=1}^{n}\sum_{j=1}^{i-1} S_{p_1\cdots p_s}(i-j)S_{q_1\cdots q_t}(j)\frac{1}{i^{m+k-a}j^a} \\
&+\sum_{a=1}^{m}\binom{k+m-1-a}{k-1}\sum_{i=1}^{n}\sum_{j=1}^{i-1} S_{p_1\cdots p_s}(j)S_{q_1\cdots q_t}(i-j)\frac{1}{i^{m+k-a}j^a} \qquad (79)
\end{aligned}$$

Now the innermost sum is of a simpler type. Hence eventually one can do this sum, and after that all remaining sums are rather simple. Therefore this defines a useful recursion. When a negative value of m or a factor $(-1)^i$ is involved things are only marginally more complicated. This algorithm has been programmed in FORM and carries the name sumnmii. An example of its application is

```
#-
#include nndecl.h
.global
L F = sum(j,1,n-1)*S(R(1,2,1),n-j)*S(R(-2,-1,-2),j)/j^2;
#call sumnmii()
.end
```

with the output

```
Time =       0.28 sec    Generated terms =       478
                F        Terms in output =       208
                         Bytes used      =      9148
```

which are all terms with a single function of weight 11.

The algorithm for doing the sums of the type

$$G^{q_1\cdots q_t}_{p_1\cdots p_s}(k,n) = -\sum_{i=1}^{n-1}(-1)^i\binom{n}{i}\frac{S_{p_1\cdots p_s}(n-i)S_{q_1\cdots q_t}(i)}{i^k} \qquad (80)$$

is more complicated. First one has to assume that all p_j and q_j are positive. Assuming also that $k \geq 0$, one can derive

$$
\begin{aligned}
G^{q_1\cdots q_t}_{mp_1\cdots p_s}(k,n) &= G^{q_1\cdots q_t}_{mp_1\cdots p_s}(k,n-1) + \frac{1}{n}G^{q_1\cdots q_t}_{mp_1\cdots p_s}(k-1,n) \\
&+\frac{1}{n}\sum_{i=1}^{n}(-1)^{i+1}\binom{n}{i}\frac{S_{p_1\cdots p_s}(n-i)S_{q_1\cdots q_t}(i)}{(n-i)^{m-j}i^k}
\end{aligned} \tag{81}
$$

Because the weight of the G-function in the second term is one less, and because one can partial fraction the last term in the end all terms have a sum over a combination with a lower weight. This means that one can use this equation for a recursion, provided one knows how to deal with the case $k = 0$ which is not handled by the above equation. For $k = 0$ one obtains after some algebra

$$
\begin{aligned}
G^{m_2q_1\cdots q_t}_{m_1p_1\cdots p_s}(0,n) &= +\frac{1}{n}\sum_{i=1}^{n}(-1)^{i+1}\binom{n}{i}\frac{S_{m_1p_1\cdots p_s}(n-i)S_{q_1\cdots q_t}(i)}{i^{m_2-1}} \\
&+\frac{1}{n}\sum_{i=1}^{n}(-1)^{i+1}\binom{n}{i}\frac{S_{p_1\cdots p_s}(n-i)S_{m_2q_1\cdots q_t}(i)}{(n-i)^{m_1-1}}
\end{aligned} \tag{82}
$$

Hence also here the weight has been decreased and one can use it for a recursion. The final expression for G can be obtained by an extra sum, because $G(k,0) = 0$ for all indices and one obtains an expression for $G(k,n) - G(k,n-1)$. One should also realize that in some cases it is necessary to change the direction of the sum ($i \to n-i$) which will introduce terms of the type $(-1)^n$ and hence this last sum can give S-functions with a negative index.

The routine that implements these algorithms (sumnmic) is a bit lengthy. A test run gives

```
#-
#include nndecl.h
.global
L  F = sum(j,1,n)*sign(j)*bino(n,j)*S(R(1,2,1),n-j)*S(R(2,1,2),j)/j^2;
#call sumnmic()
.end
```

with the result

```
Time =       0.36 sec    Generated terms =       238
                F        Terms in output =       131
                         Bytes used      =      6478
```

and a simpler example gives

```
#-
#include nndecl.h
.global
L F = sum(j,1,n)*sign(j)*bino(n,j)*S(R(2),n-j)/j;
#call sumnmic()
Print;
.end

   F =
       - S(R(-3),n) - 2*S(R(-2,1),n) - S(R(1,2),n) - S(R(2,1),n)
       - S(R(3),n);
```

D Some sums to infinity

There are special classes of sums for which the upper bound is infinity. A number of them can be evaluated to any level of complexity. Consider for instance the following sum (with $p_1 > 0$; negative values just give extra powers of -1):

$$F(m) = \sum_{j=1}^{\infty} \frac{S_{p_1\cdots p_r}(j+m)}{j^k} \tag{83}$$

Such sums can be evaluated by setting up a sum over m:

$$\begin{aligned} F(m) &= F(m-1) + \sum_{j=1}^{\infty} \frac{S_{p_2\cdots p_r}(j+m)}{(m+j)^{p_1} j^k} \\ &= F(m-1) + \sum_{i=1}^{p_1} \binom{p_1+k-1-i}{k-1} \frac{1}{m^{p_1+k-i}} (S_{i,p_2,\cdots,p_r}(\infty) - S_{i,p_2,\cdots,p_r}(m)) \\ &\quad + \sum_{i=1}^{k} \binom{p_1+k-1-i}{p_1-1} \frac{(-1)^{p_1+k-i}}{m^{p_1+k-i}} \sum_{j=1}^{\infty} \frac{S_{p_2\cdots p_r}(j+m)}{j^i} \end{aligned} \tag{84}$$

The sum in the last term is of the same type as the original sum, but it is of a simpler nature. The sum over i can just be worked out, because k and p_1 are just numbers. Hence this defines a recursion which can be worked out, if not by hand, then by computer. In the end one obtains an expression for $F(m) - F(m-1)$ which can be summed:

$$\begin{aligned} F(m) &= F(0) + \sum_{i=1}^{m} (F(i) - F(i-1)) \\ &= S_{kp_1\cdots p_r}(\infty) + \sum_{i=1}^{m} (F(i) - F(i-1)) \end{aligned} \tag{85}$$

Similarly one can consider sums of the type

$$F(m) = \sum_{j=1}^{\infty} \frac{S_{p_1\cdots p_r}(j)}{(j+m)^k} \tag{86}$$

The technique to construct a recursive solution for these sums is similar. One can study the function

$$\begin{aligned} F(m) - F(m-1) &= \sum_{j=1}^{\infty} \frac{S_{p_1\cdots p_r}(j)}{(j+m)^k} - \sum_{j=0}^{\infty} \frac{S_{p_1\cdots p_r}(j+1)}{(j+m)^k} \\ &= -\frac{S_{p_1\cdots p_r}(1)}{m^k} - \sum_{j=0}^{\infty} \frac{S_{p_2\cdots p_r}(j+1)}{(j+1)^{p_1}(j+m)^k} \\ &= -\frac{S_{p_1\cdots p_r}(1)}{m^k} - \sum_{i=1}^{p_1} \binom{p_1+k-1-i}{k-1} \frac{(-1)^{p_1+k-i}}{(m-1)^{p_1+k-i}} S_{i,p_2,\cdots,p_r}(\infty) \\ &\quad - \sum_{i=1}^{k} \binom{p_1+k-1-i}{p_1-1} \frac{1}{(m-1)^{p_1+k-i}} \sum_{j=0}^{\infty} \frac{S_{p_2\cdots p_r}(j+1)}{(j+m)^i} \end{aligned} \tag{87}$$

and again the last term is of a simpler nature. Hence there is a useful recursion and these sums can be solved.

In both cases there will be some S-functions in the answer that have the argument infinity. These should not present any special problems as they have been discussed before.

E Miscellaneous Sums

In this section some sums are given that can be worked out to any level of complexity, but they are not representing whole classes. Neither is there any proof for the algorithms. The algorithms presented have just been checked up to some rather large values of the parameters.

The sums that are treated here involve two binomial coefficients. There are quite a few of these sums in appendix F, but here are the ones that can be done to any order. The first relation that is needed is:

$$\sum_{j=0}^{m}(-1)^j\binom{m+i+j}{i+j}\binom{m+2i+j}{m+i+j} = (-1)^m\binom{m+i}{i}\binom{m+2i}{i} \tag{88}$$

Taking $m = n-i$ leads to:

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{n+j}{m+j}f^C(m+j) = -(-1)^{n+m}\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{n+j}{m+j}f(m+j) \tag{89}$$

for $0 \le m \le n$. Here f^C indicates the conjugation of appendix B. This is a rather useful identity as it divides the necessary amount of work by two. Alternatively it may even make terms cancel and hence make further evaluation unnecessary.

A new function is needed to keep the notation short:

$$U_k(n,m) = S_k(n+m) - (-1)^k S_k(n-m) - S_k(m-1) \tag{90}$$

for $k, n \ge 0$ and $m > 0$. $U_0(n,m)$ is defined to be one.

One of the ways the harmonic series can be introduced in many calculations is by expansion of the Γ-function. At the negative side its expansion is:

$$\Gamma(-n+\epsilon) = \frac{(-1)^n}{\epsilon n!}\Gamma(1+\epsilon)(1+S_1(n)\epsilon+S_{1,1}(n)\epsilon^2+S_{1,1,1}(n)\epsilon^3+S_{1,1,1,1}(n)\epsilon^4+\cdots) \tag{91}$$

Actually these special harmonic series can be written as a sum of terms that contain only products of harmonic series with a single sum as in:

$$2S_{1,1}(n) = (S_1(n))^2 + S_2(n) \tag{92}$$

$$6S_{1,1,1}(n) = (S_1(n))^3 + 3S_1(n)S_2(n) + 2S_3(n) \tag{93}$$

$$24S_{1,1,1,1}(n) = (S_1(n))^4 + 6(S_1(n))^2S_2(n) + 8S_1(n)S_3(n) + 3(S_2(n))^2 + 6S_4(n) \tag{94}$$

Notice that the factors are related to the cycle structure of the permutation group. One can define the higher U functions by analogy:

$$2U_{1,1}(n,m) = (U_1(n,m))^2 + U_2(n,m) \tag{95}$$

$$6U_{1,1,1}(n,m) = (U_1(n,m))^3 + 3U_1(n,m)U_2(n,m) + 2U_3(n,m) \tag{96}$$

$$\begin{aligned}24U_{1,1,1,1}(n,m) = {} & (U_1(n,m))^4 + 6(U_1(n,m))^2U_2(n,m) + 8U_1(n,m)U_3(n,m) \\ & +3(U_2(n,m))^2 + 6U_4(n,m)\end{aligned} \tag{97}$$

With these definitions one can write $(0 < m \le n)$:

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{n+j}{m+j}\frac{1}{(m+j)^1} = \frac{n!\,(m-1)!}{(n+m)!} \tag{98}$$

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{n+j}{m+j}\frac{1}{(m+j)^2} = \frac{n!\,(m-1)!}{(n+m)!}\,U_1(n,m) \tag{99}$$

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{n+j}{m+j}\frac{1}{(m+j)^3} = \frac{n!\,(m-1)!}{(n+m)!}\,U_{1,1}(n,m) \tag{100}$$

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{n+j}{m+j}\frac{1}{(m+j)^4} = \frac{n!\,(m-1)!}{(n+m)!}\,U_{1,1,1}(n,m) \tag{101}$$

etc. In the case that m is zero there are different expressions:

$$\sum_{j=1}^{n}(-1)^j\binom{n}{j}\binom{n+j}{j}\frac{1}{j} = -2S_1(n) \tag{102}$$

$$\sum_{j=1}^{n}(-1)^j\binom{n}{j}\binom{n+j}{j}\frac{1}{j^2} = -4S_{1,1}(n)+2S_2(n) \tag{103}$$

$$\sum_{j=1}^{n}(-1)^j\binom{n}{j}\binom{n+j}{j}\frac{1}{j^3} = -8S_{1,1,1}(n)+4S_{1,2}(n)+4S_{2,1}(n)-2S_3(n) \tag{104}$$

$$\begin{aligned}\sum_{j=1}^{n}(-1)^j\binom{n}{j}\binom{n+j}{j}\frac{1}{j^4} &= -16S_{1,1,1,1}(n)+8(S_{1,1,2}(n)+S_{1,2,1}(n)+S_{2,1,1}(n))\\ &\quad -4(S_{1,3}(n)+S_{2,2}(n)+S_{3,1}(n))+2S_4(n)\end{aligned} \tag{105}$$

and the pattern should be clear: For $1/j^k$ there will be all functions with weight k. The ones with m nested sums have a coefficient $-(-1)^{k-m}2^m$. A recipe of a similar type is found for the following sums:

$$\sum_{j=1}^{n}(-1)^j\binom{n}{j}\binom{n+j}{j}S_1(j) = 2(-1)^nS_1(n) \tag{106}$$

$$\sum_{j=1}^{n}(-1)^j\binom{n}{j}\binom{n+j}{j}S_2(j) = -2(-1)^nS_{-2}(n) \tag{107}$$

$$\sum_{j=1}^{n}(-1)^j\binom{n}{j}\binom{n+j}{j}S_3(j) = (-1)^n(2S_{-3}(n)-4S_{-2,1}(n)) \tag{108}$$

$$\sum_{j=1}^{n}(-1)^j\binom{n}{j}\binom{n+j}{j}S_4(j) = (-1)^n(-2S_{-4}(n)+4(S_{-3,1}(n)+S_{-2,2}(n))-8S_{-2,1,1}(n)) \tag{109}$$

and the pattern here is that one should make all higher series that start with a negative index that has a value of at most -2, after which there are only positive indices. All functions are of weight k (for S_k inside the sum), and for m nested sums the coefficient is $(-1)^{n+k-m}2^m$. The exception is $k=1$ but that is because S_1 is its own associated function and its conjugate is purely of the type $1/j^k$.

F Summation tables

During the work that inspired this paper quite a few other sums were evaluated that are not represented by the above algorithms. Many of these sums can only be done for a fixed weight and most of them were not readily available in the literature. Hence they are presented here in a number of tables, even though eventually many of these sums were not needed in the final version of the program. For completeness also a large number of sums are presented that are already available in the literature. A number of these sums can be derived formally. Some were derived by 'guessing' and then trying the resulting formula for a large number of values.

In all sums it is assumed that all parameters i,j,k,l,m,n are integers and have values ≥ 0. In some cases the formulae can be extended to noninteger values.

It should be noted that all sums that can be handled by the procedures of the previous appendices are not in the tables. They would make the tables unnecessarily lengthy.

Some formulae that are used very often are presented first:

$$\sum_{i=0}^{n} \frac{(m+i)!}{i!} = \frac{(n+m+1)!}{n!(m+1)} \tag{110}$$

$$\sum_{i=0}^{n} \frac{(m+i)!}{(k+i)!} = \frac{(n+m+1)!}{(n+k)!(m+1-k)} - \frac{m!}{(k-1)!(m+1-k)} \tag{111}$$

$$\sum_{j=0}^{n} (-1)^j \binom{n}{j} = \delta(n) \tag{112}$$

$$\sum_{j=0}^{m} (-1)^j \binom{n}{j} = (-1)^m \binom{n-1}{m} \tag{113}$$

$$\sum_{j=0}^{n} \binom{n}{j} (m+j)!\,(k+n-j)! = m!\,k! \frac{(m+k+n+1)!}{(m+k+1)!} \tag{114}$$

$$\sum_{j=0}^{n} (-1)^j \binom{n}{j} \frac{(m+j)!}{(m+k+j)!} = \frac{(n+k-1)!}{(k-1)!} \frac{m!}{(m+n+k)!} \tag{115}$$

$$\sum_{j=0}^{n} (-1)^j \binom{n}{j} \binom{n+m+k+j}{m+j} = (-1)^n \binom{n+m+k}{k} \tag{116}$$

The last three formulae can be extended to noninteger values of m and k. They can be used occasionally before Γ-functions are expanded to yield harmonic series.

At times some auxiliary functions were needed. They are defined by

$$A_k(n,m) = \sum_{j=1}^{n} (-1)^j \binom{n+m}{j} \frac{1}{j^k} \tag{117}$$

$$\Delta(1,1,a,b) = \sum_{i=a}^{b} \sum_{j=a}^{a+b-i} \frac{1}{i\,j} \tag{118}$$

$$R_{m,k}(n) = \sum_{j=1}^{n} \frac{S_m(2j)}{j^k} \tag{119}$$

Sometimes Δ is not always the easiest function to manipulate. Therefore the function Δ' is sometimes handy:

$$\begin{aligned} \Delta'(1,1,a,b) &= \frac{1}{2}\theta(b-a)(\Delta(1,1,a,b) - (S_1(a-1) - S_1(b))^2) \\ &\quad -\frac{1}{2}\theta(a-b-1)\Delta(1,1,b+1,a-1) \end{aligned} \tag{120}$$

Both functions involve summations over triangles in the two dimensional plane. These triangles do not touch the origin.

F.1 Sums without $(-1)^j$

First is a number of expressions that are at the lowest level of complexity.

$$A_1(n,1) = -S_1(n+1) + \frac{(-1)^n}{n+1} \tag{121}$$

$$A_1(n,2) = -S_1(n+2) + \frac{(-1)^n}{(n+1)(n+2)} + (-1)^n \tag{122}$$

$$A_1(1,m) = -(m+1) \tag{123}$$

$$A_1(2,m) = \frac{1}{4}(m+2)(m-3) \tag{124}$$

$$A_1(n,m+1) = A_1(n,m) + (-1)^n\binom{n+m}{n}\frac{1}{n+m+1} - \frac{1}{n+m+1} \tag{125}$$

$$A_1(n+1,m) = A_1(n,m+1) - (-1)^n\binom{n+m+1}{m}\frac{1}{n+1} \tag{126}$$

$$A_k(n,m+1) = \sum_{i=1}^{k}(n+m+1)^{i-k}A_i(n,m) + \left((-1)^n\binom{n+m}{n} - 1\right)\frac{1}{(n+m+1)^k} \tag{127}$$

$$A_k(n,m+1) = A_k(n,m) + \sum_{j=1}^{n}(-1)^j\binom{n+m+1}{j}S_k(j) - (-1)^n\binom{n+m}{n}S_k(n) \tag{128}$$

Next are some miscellaneous sums:

$$\begin{aligned}\sum_{j=1}^{a}\frac{1}{j}S_1(b+j) &= (S_1(a) - S_1(b))S_1(a+b) + 2S_{1,1}(b) - \frac{1}{2}S_2(b) \\ &\quad + \Delta'(1,1,a,b)\end{aligned} \tag{129}$$

$$\sum_{j=0}^{m}\binom{n-1+j}{j}\frac{1}{n+j} = \binom{n+m}{n}\frac{1}{n} - (-1)^n A_1(n,m) - (-1)^n S_1(n+m) \tag{130}$$

$$\sum_{j=1}^{n}\frac{S_1(n+j)}{j} = 2S_{1,1}(n) - \frac{1}{2}S_2(n) \tag{131}$$

$$\sum_{j=1}^{n}\frac{S_1(j)}{n+j} = S_1(2n)S_1(n-1) - 2S_{1,1}(n-1) + \frac{1}{2}S_2(n) \tag{132}$$

$$\sum_{j=1}^{n}\frac{S_{-1}(n+j)}{j} = S_{-1,-1}(n) + S_{1,-1}(n) - \frac{1}{2}S_2(n) \tag{133}$$

$$\sum_{j=1}^{n}\frac{S_1(n+j)}{j^2} = S_{1,2}(n) - 2S_{2,1}(n) - \frac{1}{2}S_3(n) + 2R_{1,2}(n) \tag{134}$$

$$\sum_{j=1}^{n}\frac{S_{-1}(n+j)}{j^2} = 2S_{2,1}(n) - S_{-2,-1}(n) + S_{-1,-2}(n) - S_{2,-1}(n) - \frac{1}{2}S_3(n) - 2R_{1,2}(n) \tag{135}$$

$$\sum_{j=1}^{n}\frac{S_{-2}(n+j)}{j} = S_{-2,-1}(n) + S_{1,-2}(n) + S_{2,-1}(n) - S_{2,1}(n) - \frac{1}{4}S_3(n) + R_{1,2}(n) \tag{136}$$

$$\sum_{j=1}^{m}\frac{1}{n+j+2}S_1(j) = S_1(m)S_1(n+m+2) - \sum_{j=1}^{m}\frac{1}{j}S_1(n+j+1) \tag{137}$$

$$\sum_{j=1}^{m}\frac{1}{n+j+2}S_1(j+1) = -\sum_{j=1}^{m}\frac{1}{j+1}S_1(n+1+j)+S_1(m+1)S_1(n+m+2)-S_1(n+2) \tag{138}$$

The last two equations are not solving anything, but they are useful in the derivation of some of the next sums. First an equation that is like a partial integration.

$$\sum_{j=0}^{n}\binom{m+j}{j}f(n+1-j) = \sum_{j=0}^{n}\binom{m-1+j}{j}\sum_{i=1}^{n+1-j}f(i) \tag{139}$$

It is central in the derivation of the next equations

$$\sum_{j=0}^{n}\binom{m+j}{j}\frac{1}{n+1-j} = \binom{n+m+1}{n+1}(S_1(n+m+1)-S_1(m)) \tag{140}$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{m+j}{j}\frac{1}{(n+1-j)^2} &= \binom{n+m+1}{n+1}(S_1(n+1)(S_1(n+m+1)-S_1(m-1)) \\ &\quad +2S_2(n+m+1)-2S_{1,1}(n+m+1)+\sum_{i=1}^{m-1}\frac{S_1(n+m+1-i)}{i})\end{aligned} \tag{141}$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{m+j}{j}S_k(n+1-j) &= \frac{n+m+2}{m+1}\sum_{j=0}^{n}\binom{m+j-1}{j}S_k(n+1-j) \\ &\quad -\frac{1}{m+1}\sum_{j=0}^{n}\binom{m+j-1}{j}S_{k-1}(n+1-j)\end{aligned} \tag{142}$$

$$\sum_{j=0}^{n}\binom{m+j}{j}S_1(n+1-j) = \binom{n+m+2}{n+1}(S_1(n+m+2)-S_1(m+1)) \tag{143}$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{m+j}{j}S_{1,1}(n+1-j) &= \frac{1}{2}\binom{n+m+2}{n+1}(2S_{1,1}(m+1)-2S_{1,1}(n+1)+S_2(n+1) \\ &\quad -\frac{1}{(n+m+2)(m+1)}-\Delta'(1,1,m,n+1)-\Delta'(1,1,m+1,n+1) \\ &\quad +(2S_1(n+m+2)-\frac{1}{n+m+2})(S_1(n+1)-S_1(m+1))\ )\end{aligned} \tag{144}$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{m+j}{j}S_2(n+1-j) &= \binom{n+m+2}{n+1}(S_2(n+m+2)-S_{1,1}(n+m+2) \\ &\quad +S_1(n+m+1)S_1(n+1)+\frac{S_1(m)}{n+m+2}+\frac{1}{2}S_2(n+1) \\ &\quad -S_{1,1}(n+1)-\Delta'(1,1,m,n+1)\ )\end{aligned} \tag{145}$$

Similarly one can derive:

$$\sum_{j=0}^{n}\binom{m+j}{j}S_1(m+j) = \binom{n+m+1}{n}(S_1(n+m+1)-\frac{1}{m+1}) \tag{146}$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{m+j}{j}S_1^2(m+j) &= \binom{n+m+1}{n}((S_1(n+m)-\frac{1}{m+1})(\frac{1}{n+m+1}-\frac{1}{m+1}) \\ &\quad +S_{1,1}(n+m))-(-1)^m\frac{1}{m+1}(S_1(n+m)+A_1(m,n))\end{aligned} \tag{147}$$

$$\sum_{j=0}^{n} \binom{m+j}{j} S_2(m+j) = \binom{n+m+1}{n} S_2(n+m) - \frac{(-1)^m}{m+1}(S_1(n+m) + A_1(m,n)) \tag{148}$$

These formulae give also some 'partial integration':

$$\begin{aligned}\sum_{j=0}^{n-1} \frac{(m+j)!}{j!} S_1(m+j) f(n-j) &= \sum_{j=0}^{n-1} m \frac{(m+j-1)!}{j!} S_1(m+j-1) \sum_{i=1}^{n-j} f(i) \\ &+ \sum_{j=0}^{n-1} \frac{(m+j)!}{j!\, m} f(n-j) \end{aligned}\tag{149}$$

$$\begin{aligned}\sum_{j=0}^{n} \frac{(m-1+j)!}{j!} S_1(m+j) f(n+1-j) &= -(m-1) \sum_{j=0}^{n+1} \frac{(m-2+j)!}{j!} S_1(m-1+j) f(n+2-j) \\ &+ \sum_{j=0}^{n+1} \frac{(m-1+j)!}{j!} S_1(m-1+j) f(n+2-j) \end{aligned}\tag{150}$$

This is used for the next equations

$$\begin{aligned}\sum_{j=0}^{n-1} \binom{m+j}{j} \frac{S_1(m+j)}{n-j} &= \binom{m+n}{n}(2S_{1,1}(m+n) - 2S_2(m+n) \\ &+ S_2(m) - S_1(m+n)S_1(m)) \end{aligned}\tag{151}$$

$$\begin{aligned}\sum_{j=0}^{n-1} \binom{m+j}{j} S_1(m+j) S_1(n-j) &= \binom{n+m+1}{n}(-(S_2(n+m+1) - S_2(m+1)) \\ &+ (S_1(n+m+1) - S_1(m+1))(S_1(n+m+1) - \frac{1}{m+1})) \end{aligned}\tag{152}$$

F.2 Sums with $(-1)^j$

The next sums all contain a factor $(-1)^j$ and hence they give completely different results than the corresponding set of sums without the $(-1)^j$. The most important ones have been treated in the appendices B and C.

$$\sum_{j=0}^{n} \binom{n}{j} (-1)^j \frac{1}{m+j} = \binom{n+m}{n}^{-1} \frac{1}{m} \tag{153}$$

$$\sum_{j=0}^{n} \binom{n}{j} (-1)^j S_1(m+j) = -\binom{n+m}{n}^{-1} \frac{1}{n} \tag{154}$$

$$\sum_{j=0}^{n} \binom{n}{j} (-1)^j \frac{1}{(m+j)^2} = \binom{n+m}{n}^{-1} \frac{1}{m}(S_1(m+n) - S_1(m-1)) \tag{155}$$

$$\sum_{j=0}^{n} \binom{n}{j} (-1)^j \frac{S_1(m+j)}{m+j} = \binom{n+m}{n}^{-1} \frac{1}{m}(S_1(m+n) - S_1(n)) \tag{156}$$

$$\sum_{j=0}^{n} \binom{n}{j} (-1)^j S_2(m+j) = -\binom{n+m}{n}^{-1} \frac{1}{n}(S_1(n+m) - S_1(m)) \tag{157}$$

$$\sum_{j=0}^{n} \binom{n}{j} (-1)^j S_{1,1}(m+j) = -\binom{n+m}{n}^{-1} \frac{1}{n}(S_1(n+m) - S_1(n-1)) \tag{158}$$

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\frac{S_1(n-j)}{m+j} = -A_1(n,m)\left((n+m)\binom{n+m-1}{n}\right)^{-1} \tag{159}$$

There is also a number of sums with more than one binomial coefficient. First a few general ones.

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{m+j}{j} = (-1)^n\binom{m}{n} \quad m \geq n \tag{160}$$

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{m+j}{j} = 0 \quad m < n \tag{161}$$

$$\begin{aligned}\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{m+j}{j}\, j &= (-1)^n\binom{m+1}{n}\, n \quad m \geq n-1 \\ &= 0 \qquad\qquad m < n-1\end{aligned} \tag{162}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{m+j}(-1)^j = 0 \quad 0 < m < n \tag{163}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+m+j}{m+j}(-1)^j = (-1)^n \quad m \geq 0 \tag{164}$$

$$\sum_{j=0}^{n}\frac{1}{j!(n+1-j)!}\frac{(2n+2-j)!}{(n+1-j)!}(-1)^j = 1+(-1)^n \tag{165}$$

$$\sum_{j=0}^{n-1}\frac{1}{j!(n-1-j)!}\frac{(n-1+j)!}{j!(j+2)}(-1)^j = \frac{1}{2}\delta(n-1) - \frac{1}{6}\delta(n-2) \tag{166}$$

And now the sums with two binomial coefficients and an argument j in the extra piece (see also appendix E):

$$\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j S_{1,1}(j) = (-1)^n(4S_{1,1}(n) - 2S_2(n)) \tag{167}$$

$$\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j \frac{1}{j}S_1(j) = 2S_{-2}(n) \tag{168}$$

$$\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j S_{1,2}(j) = (-1)^n(2S_{-3}(n) - 4S_{1,-2}(n)) \tag{169}$$

$$\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j S_{2,1}(j) = (-1)^n(2S_3(n)) \tag{170}$$

$$\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j S_{1,1,1}(j) = (-1)^n(2S_3(n) - 4S_{1,2}(n) - 4S_{2,1}(n) + 8S_{1,1,1}(n)) \tag{171}$$

$$\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j \frac{1}{j}S_2(j) = -2S_3(n) \tag{172}$$

$$\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j \frac{1}{j}S_{1,1}(j) = 4S_{-2,1}(n) - 2S_{-3}(n) \tag{173}$$

$$\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j \frac{1}{j^2}S_1(j) = 4S_{1,-2}(n) - 2S_{-3}(n) \tag{174}$$

Similarly there are formulae with $j+1$ (see also appendix E).

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+1}(-1)^j S_1(j+1) = (-1)^n \frac{1}{n+1} \tag{175}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+1}(-1)^j \frac{S_1(j+1)}{j+1} = -(-1)^n \frac{1}{n(n+1)^2} \tag{176}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+1}(-1)^j S_{1,1}(j+1) = \frac{(-1)^n}{n+1}(S_1(n+1)+S_1(n-1)) \tag{177}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+1}(-1)^j S_2(j+1) = -\frac{1}{n(n+1)^2} \tag{178}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+1}(-1)^j \frac{S_1(j+1)}{(j+1)^2} = -\frac{1}{n+1}(S_{-2}(n+1)+S_{-2}(n-1)+\frac{(-1)^n}{n(n+1)}) \tag{179}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+1}(-1)^j \frac{S_{1,1}(j+1)}{j+1} = \frac{(-1)^n}{n(n+1)^2}(1-S_1(n+1)-S_1(n-1)) \tag{180}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+1}(-1)^j \frac{S_2(j+1)}{j+1} = \frac{1}{n^2(n+1)^2}+\frac{1}{(n+1)^3} \tag{181}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+1}(-1)^j S_3(j+1) = \frac{1}{n(n+1)^2}(1-S_1(n+1)-S_1(n-1)) \tag{182}$$

And the formulae with $j+2$ (see also appendix E).

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+2}(-1)^j S_1(j+2) = -(-1)^n \frac{1}{(n+1)(n+2)} \tag{183}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+2}(-1)^j S_2(j+2) = -\frac{2(n^2+n+1)}{(n-1)n(n+1)^2(n+2)^2} \tag{184}$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+2}(-1)^j S_3(j+2) &= \frac{1}{(n+1)(n+2)}(\frac{11/6}{n-1}-\frac{5/2}{n}+\frac{5/2}{n+1}-\frac{11/6}{n+2}+(-1)^n \times \\ &\quad \times(S_1(n+2)+S_1(n-2))(S_{-1}(n+2)-S_{-1}(n-2))\ )\end{aligned} \tag{185}$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j+2}(-1)^j \frac{S_2(j+2)}{j+2} &= \frac{1}{(n+1)(n+2)}(S_2(n+2)-S_2(n-2) \\ &\quad -\frac{5}{6}\frac{1}{n-1}+\frac{1}{2}\frac{1}{n}-\frac{1}{2}\frac{1}{n+1}+\frac{5}{6}\frac{1}{n+2})\end{aligned} \tag{186}$$

The formulae with $j+n$:

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j \frac{1}{n+j} = 0 \tag{187}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j S_1(n+j) = 2(-1)^n S_1(n) \tag{188}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j \frac{1}{(n+j)^2} = -(-1)^n \frac{(n-1)!(n-1)!}{(2n)!} \tag{189}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j(S_{1,1}(n+j)-S_2(n+j)) = (-1)^n(4S_{1,1}(n)-3S_2(n)) \quad (190)$$

$$\sum_{j=1}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j\frac{1}{j}S_1(n+j) = 3S_2(n)+2S_{-2}(n)-4S_{1,1}(n) \quad (191)$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j\frac{1}{j+1}S_1(n+j) = (-1)^n\frac{1}{n(n+1)} \quad (192)$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{1+j}(-1)^jS_1(n+j) = (-1)^n\frac{1}{n+1} \quad (193)$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{1+j}(-1)^jS_2(n+j) = (-1)^n\frac{n!\,(n-1)!}{(2n)!}\frac{1}{n+1} \quad (194)$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{2+j}(-1)^jS_2(n+j) = (-1)^n\frac{n!\,(n-1)!}{(2n)!}\left(\frac{1}{3}\frac{1}{n+2}-\frac{1}{n+1}-\frac{1}{3}\frac{1}{n-1}\right) \quad (195)$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{3+j}(-1)^jS_2(n+j) &= (-1)^n\frac{n!\,(n-1)!}{(2n)!}\left(\frac{1}{10}\frac{1}{n+3}-\frac{2}{3}\frac{1}{n+2}\right.\\ &\quad\left.+\frac{1}{n+1}+\frac{1}{6}\frac{1}{n-1}+\frac{2}{5}\frac{1}{n-2}\right) \quad (196)\end{aligned}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j\frac{1}{(j+1)^2}S_1(n+j) = \frac{1}{n(n+1)}S_1(n-1)-(-1)^n\frac{1}{n^2(n+1)^2} \quad (197)$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j\frac{1}{j+2}S_1(n+j) = (-1)^n\left(\frac{1}{6}\frac{1}{n-1}+\frac{1}{2}\frac{1}{n}-\frac{1}{2}\frac{1}{n+1}-\frac{1}{6}\frac{1}{n+2}\right) \quad (198)$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{2+j}(-1)^j\frac{1}{j+2}S_1(n+j) = \frac{n!}{(n+2)!}\left(S_1(n-2)+2(-1)^n(n^2+n+1)\frac{(n-2)!}{(n+2)!}\right) \quad (199)$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{3+j}(-1)^j\frac{1}{j+3}S_1(n+j) = \frac{2\;n!}{(n+3)!}\left(S_1(n-3)-(S_{-1}(n+3)-S_{-1}(n-3))\right) \quad (200)$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{1+j}(-1)^j\frac{1}{(j+1)^2}S_1(n+j) &= \frac{1}{n+1}\left(2S_{1,1}(n-1)-2S_2(n-1)-S_{-2}(n+1)\right.\\ &\quad\left.-S_{-2}(n-1)+S_1(n+1)S_1(n-1)-\frac{(-1)^n}{n(n+1)}\right) \quad (201)\end{aligned}$$

$$\begin{aligned}\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{2+j}(-1)^j\frac{1}{(j+2)^2}S_1(n+j) &= \frac{n!}{(n+2)!}\left(2S_{1,1}(n-2)-2S_2(n-2)-S_1(n-2)\right.\\ &\quad-S_{-2}(n+2)-S_{-2}(n-2)+S_1(n+2)S_1(n-2)\\ &\quad\left.+(-1)^n(n^2+n+3)\frac{(n-2)!}{(n+2)!}\right) \quad (202)\end{aligned}$$

And some mixed formulae.

$$\begin{aligned}\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j\frac{1}{m+j} &= 0 \qquad (m\le n)\\ &= (-1)^n\frac{(m-1)!(m-1)!}{(n+m)!(m-n-1)!} \qquad (m>n) \quad (203)\end{aligned}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{j}(-1)^j\frac{1}{(m+j)^2} = -(-1)^m\frac{(m-1)!(m-1)!(n-m)!}{(n+m)!} \quad (n\geq m) \tag{204}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{m+j}(-1)^j S_2(m+j) = (-1)^{n+m}\frac{(m-1)!\;n!}{(n+m)!}(S_{-1}(n+m)-S_{-1}(n-m)) \quad (n\geq m) \tag{205}$$

$$\sum_{j=0}^{n}\binom{n}{j}\binom{n+j}{m+j}(-1)^j S_1(n+j) = -(-1)^{n+m}\frac{n!\;(m-1)!}{(n+m)!} \quad (n\geq m) \tag{206}$$

There are also sums with two factorials in the numerator.

$$\sum_{j=0}^{n} j!(m-j)!(-1)^j = \frac{(m+1)!}{m+2}+(-1)^n\frac{(n+1)!\;(m-n)!}{m+2} \tag{207}$$

$$\sum_{j=1}^{n} j!\;(m-j)!(-1)^j S_1(j) = (-1)^n\frac{(n+1)!\;(m-n)!}{m+2}(S_1(n+1)-\frac{1}{m+2}) -\frac{(m+1)!}{(m+2)^2} \tag{208}$$

$$\sum_{j=0}^{n} j!\;(n-j)!(-1)^j\frac{1}{j+1} = -(n+1)!\;(S_2(n+1)+2S_{-2}(n+1)) \tag{209}$$

$$\sum_{j=1}^{n} j!\;(n-j)!(-1)^j\frac{1}{j^2} = n!\;(S_2(n)+2S_{-2}(n)) \tag{210}$$

$$\sum_{j=0}^{m}(-1)^j j!\frac{(n+m-j)!}{2+m-j} = (-1)^m(m+2)!\;(n-2)!\;(A_1(m+3,n-2)+S_1(m+2)) +\frac{(m+n+1)!}{(m+3)^2}+(-1)^m(m+1)!\;(n-1)! \tag{211}$$

$$\sum_{j=0}^{n}(-1)^j(n+m-j)!\;j!\;A_1(j,n-j) = \frac{(n+m+1)!}{n+m+2}(S_1(n+m+1)-S_1(m+1)) -(-1)^n\frac{(n+1)!\;m!}{n+m+2}S_1(n) \tag{212}$$

F.3 Partial sums

For derivations the use of partial sums (sums of only part of the range of the binomial coefficients) are very useful. Unfortunately these are hard to obtain and hence only a limited number of them can be presented here.

$$\sum_{j=0}^{m}(-1)^j\binom{n}{j} = (-1)^m\binom{n-1}{m} \tag{213}$$

$$\sum_{j=1}^{m}(-1)^j\binom{n}{j}\frac{1}{j^k} = A_k(m,n-m) \tag{214}$$

$$\sum_{j=0}^{m}(-1)^j\binom{n}{j}S_1(j) = (-1)^m\binom{n-1}{m}(S_1(m)+\frac{1}{n})-\frac{1}{n} \tag{215}$$

$$\sum_{j=0}^{m}(-1)^j\binom{n}{j}S_1(n-j) = (-1)^m\binom{n-1}{m}(S_1(n-m-1)+\frac{1}{n}) \tag{216}$$

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