Iterated integrals over letters induced by quadratic forms

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An automated treatment of iterated integrals based on letters induced by real-valued quadratic forms and Kummer–Poincaré letters is presented. These quantities emerge in analytic single and multiscale Feynman diagram calculations. To compactify representations, one wishes to apply general properties of these quantities in computer-algebraic implementations. We provide the reduction to basis representations, expansions, analytic continuation and numerical evaluation of these quantities.

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I. INTRODUCTION

In analytic calculations of single and multiscale Feynman integrals different principal structures have been revealed in particular during the last 30 years.1 Beyond the multiple zeta values [2] and other special numbers for zero-scale quantities, there are the spaces of harmonic sums [3,4], harmonic polylogarithms [5], generalized harmonic sums [6,7] and Kummer–Poincaré iterated integrals [6–8], cyclotomic harmonic sums and iterated integrals [9], finite and infinite binomial sums and inverse binomial sums and the associated root-letter integrals [10,11], and iterative non–iterative integrals [12], including those containing complete elliptic integrals [12,13]. This list is expected still to extend in analytic calculations at even higher loops and for more contributing scales in the future.

In decomposing Feynman parameter representations in the general case, cf., e.g., [14], often real polynomials of higher degree have to be factored. According to the fundamental theorem of algebra [15] this leads to either linear and quadratic factors in real representations or to linear complex-valued factors with conjugated pairs. Real representations have often advantages in calculations. This is the main reason to extend the class of Kummer–Poincaré iterated integrals based on the alphabet

\[ \mathfrak{A}_R = \left\{ \frac{1}{x - c_i} \left| c_i \in \mathbb{C} \right. \right\} \]  

(1.1)

\[ \mathfrak{A}_{KP} = \left\{ \frac{1}{x - c_i} \left| c_i \in \mathbb{C} \right. \right\} \]

1For a survey see [1].

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\[ \frac{d}{dz} H_{b,\vec{a}}(z) = f_b(z) H_{\vec{a}}(z), \]  

(1.4)

There is an overlap with the cyclotomic iterated integrals [9] with respect to the letters 1/\(\Phi_k(x)\), \(k = 3, 4, 6\). The associated iterative integrals are given by

\[ H_{b,\vec{a}}(z) = \int_0^z dx f_b(x) \Phi_k(x), \quad H_{\emptyset} = 1, \quad f_i(x) \in \mathfrak{A}_R. \]  

(1.3)

Iterated integrals do also obey the differential property

\[ x^2 + b_i x + c_i \text{ is irreducible over } \mathbb{R}. \]
simple main variable. This has the advantage that the corresponding results can be iterated over in further integrations, which will be necessary for the use in a higher order calculation.

Using iterative integrals in the description of physical quantities it is required to give them a clear definition. In some cases it is possible that a first definition has singularities in subintegrals, which have to be dealt with to obtain a measurable quantity. Furthermore, the real and imaginary parts of the respective integrals have to be separated from the beginning, because they have a different physical meaning and it then allows to deal with real integrals only. One has also to observe that certain transformations in the main argument may effect the position of cuts chosen. In the case of singularities of the real integrals we will apply Cauchy’s principal value for definiteness, as it is also the case in amplitudes referring to the Källén–Lehmann representation [18].

In Sec. II we will describe the different operations for the iterated integrals induced by quadratic forms in the package {\textsc{Harmonicsums}} [3–5,7,9,10,19–21] and provide test examples. Section III deals with integrals of a recent physical application [16] which we reconsider in the present formalism, and Sec. IV contains the conclusion.

II. OPERATIONS FOR THE ITERATED INTEGRALS

In the following we describe a series of operations which allow to deal with iterated integrals containing letters of the alphabet $\mathbb{A}_R$. The statement

\[ \text{QL}[\{(a_1,b_1,c_1),d_1\},\{(a_2,b_2,c_2),d_2\},\{(a_3,b_3,c_3),d_3\},z] \]  

represents the integral

\[ H((a_1,b_1,c_1),d_1,((a_2,b_2,c_2),d_2),((a_3,b_3,c_3),d_3))(z) = \int_0^z \int_0^{t_1} \int_0^{t_2} (a_1 + b_1 t_1 + c_1 t_1^2) (a_2 + b_2 t_2 + c_2 t_2^2) (a_3 + b_3 t_3 + c_3 t_3^2), \]

with $d_i \in \{0,1\}, a_i, b_i, c_i \in \mathbb{R}$,

covering a number of iterated letters out of $\mathbb{A}_R$. The command \text{ToHarmonicSumsIntegrate} reveals the integral structure in explicit form. One may convert these integrals into GL–functions, cf. [10], by \text{QLToGL} and GL–functions with letters out of $\mathbb{A}_R$ to QL–functions by \text{GLToQL}.

It is allowed that the Kummer–Poincaré letters in $\mathbb{A}_{Kp}$ have poles in the integration region. The iterative integral is then defined taking Cauchy’s principal value. However, the quadratic denominators are assumed to not factorize in real numbers.

The numerical evaluation of QL–functions is performed as in the following example

\[ r = \text{ToHarmonicSumsIntegrate}[\text{QL}[\{(1,1,2),1\},\{(1,-1,1),1\},\{(-1,1,1),1\},\frac{1}{2}], \]

\[ \text{NIntegrate} \rightarrow \text{True}]//\text{ReleaseHold} \]

\[ r \approx -0.0000649218. \]

Here not all letters corresponding to quadratic forms are yet in the standard form. There is no singularity, however, in the integration region since $(\sqrt{5} - 1)/2 > 1/2$.

To be able to deal with properly defined letters, the mapping \text{QLToStandardForm} is used. A typical example is

\[ \text{QL}[\{(1,1,2),2\},z] = \int_0^z dt \frac{t^2}{1 + t + 2t^2} \]

\[ \text{QLToStandardForm}[\text{QL}[\{(1,1,2),2\},z]] \Rightarrow \frac{z}{2} - \frac{1}{4} \int_0^z dt \frac{1}{\frac{3}{2} + \frac{3}{2} + t^2} - \frac{1}{4} \int_0^z dt \frac{t}{\frac{3}{2} + \frac{3}{2} + t^2}. \]
The shuffle operation is

\[ H_{a_1, \ldots, a_n}(z) \cdot H_{b_1, \ldots, b_m}(z) = H_{a_1, \ldots, a_n} \cup H_{b_1, \ldots, b_m}(z) = \sum_{c_i \in \{a_1, \ldots, a_n \cup b_1, \ldots, b_m\}} H_{c_i}(z), \quad (2.7) \]

where all combinations of the two index sets are allowed, which preserve the ordering in these two sets. Here \( H \) labels a general iterated integral. The corresponding command is \texttt{LinearHExpand}.

One obtains

\[ \text{LinearHExpand} \left[ QL \left[ \left\{ \left\{ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right\}, 0 \right\} \right] \right], \quad (2.8) \]

The algebraic reduction with respect to shuffle relations of a given expression is performed by the command \texttt{ReduceToQLBasis}, which will also transform the shuffled expression \((2.8)\) into the corresponding product expression. Often one would like to remove trailing indices or leading indices of QL-functions. This is done by the commands \texttt{RemoveTrailing0}, \texttt{RemoveTrailingIndex} or \texttt{RemoveLeading1}, \texttt{RemoveLeadingIndex}. Here \texttt{Trailing0} refers to the letter \(1/x\) and \texttt{Leading1} to \(1/(1 - x)\). Examples are

\[ \text{RemoveTrailingIndex} [QL][\{\{1,1,1,0\},\{-1,1,0\},\{1,1,1,0\},\{1,1,1,0\},z],[\{1,1,1,0\}] \]

\[ = \frac{1}{2} QL[\{\{1,1,1,0\},\{1,1,1,0\},\{-1,1,0\},\{1,1,1,0\},z] \]

\[ - 2QL[\{\{1,1,1,0\},\{-1,1,0\},\{1,1,1,0\},\{-1,1,0\},z] \]

\[ + 3QL[\{\{1,1,1,0\},\{1,1,1,0\},\{1,1,1,0\},\{-1,1,0\},\{1,1,1,0\},z]. \quad (2.9) \]

\[ \text{RemoveLeadingIndex} [QL][\{\{1,1,1,0\},\{-1,1,0\},\{1,1,1,0\},\{-1,1,0\},z],[\{1,1,1,0\}] \]

\[ = QL[\{\{1,1,1,0\},\{-1,1,0\},\{1,1,1,0\},z],[\{1,1,1,0\}] \]

\[ - 2QL[\{-1,1,0\},\{1,1,1,0\},\{1,1,1,0\},\{-1,1,0\},\{-1,1,0\},z]. \quad (2.10) \]

The series expansion of the QL-function about \( z = 0 \) is obtained by the command \texttt{QLSeries}, e.g.,

\[ \text{QLSeries} \left[ QL \left[ \left\{ \left\{ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right\}, 0 \right\} \right] \right], 10 \]

\[ = \frac{z^5}{45} - \frac{z^6}{216} + \frac{11 z^7}{1260} + \frac{13 z^8}{1620} - \frac{7 z^9}{972} + \frac{4793 z^{10}}{680400}. \quad (2.11) \]

or

\[ \text{QLSeries} [QL][\{\{1,1,1,1\},\{3,1,1,0\},\{0,1,0,0\},z],[z],5] \]

\[ = -\frac{4 z^3}{27} + \frac{11 z^4}{96} - \frac{5 z^5}{972} + \left[ \frac{z^3}{72} - \frac{7 z^4}{162} + \frac{z^5}{162} \right] \ln(z). \quad (2.12) \]

Often a change in the argument of the QL-functions is desirable. The following transformations are implemented and are carried out by the command \texttt{TransformQL}
\[ k \cdot z \rightarrow z, \quad k \in \mathbb{Q}, \quad 1 - z \rightarrow z, \quad \frac{1}{z} \rightarrow z, \quad \frac{1 - z}{1 + z} \rightarrow z. \] 

(2.13)

Examples are

\[
\text{TransformQL} \left[ \{\{1, 1, 1\}, \{2, 1, 1\}, 0\}, 2z, z \right] \Rightarrow \frac{1}{2} \text{QL} \left[ \begin{array}{c} \{\{1, 1, 1\}, 1\}, \{\{\frac{1}{2}, 0\}, 1\}, \{\{\frac{1}{2}, 0\}, 0\} \end{array} \right] \cdot x, \]

(2.14)

\[
\text{TransformQL} \left[ \{\{1, 1, 1\}, \{2, 1, 1\}, 0\}, 1 - z, z \right] \\
\Rightarrow \text{QL} \left[ \{\{2, 1, 1\}, 0\}, 1 \right] - \text{QL} \left[ \{\{3, 3, 1\}, 0\}, z \right] + \text{QL} \left[ \{\{3, 3, 1\}, 1\}, z \right] \\
+ \text{QL} \left[ \{\{1, 1, 1\}, \{2, 1, 1\}, 0\}, 1 \right] + \text{QL} \left[ \{\{3, 3, 1\}, 0\}, \{\{4, 3, 1\}, 0\}, z \right] \\
- \text{QL} \left[ \{\{3, 3, 1\}, \{4, 3, 1\}, 0\}, z \right].
\]

(2.15)

\[
\text{TransformQL} \left[ \{\{1, 1, 1\}, \{2, 1, 1\}, 0\}, \frac{1}{z}, z \right] \\
\Rightarrow \left[ -\text{QL} \left[ \{\{0, 1, 0\}, 0\}, z \right] - \text{QL} \left[ \{\{1, 1, 1\}, 0\}, 1 \right] + \text{QL} \left[ \{\{1, 1, 0\}, 0\}, z \right] \right] + \frac{1}{2} \text{QL} \left[ \left\{\{\frac{1}{2}, 1\}, 0\right\}, 1 \right] \\
+ 2 \text{QL} \left[ \{\{2, 1, 1\}, 0\}, 1 \right] - \text{QL} \left[ \{\{0, 1, 0\}, \left\{\frac{1}{2}, 1\right\}, 0\right\}, 1 \right] \\
+ \text{QL} \left[ \left\{\{0, 1, 0\}, \left\{\frac{1}{2}, 1\right\}, 0\right\}, z \right] + \text{QL} \left[ \left\{\{1, 1, 1\}, \left\{\frac{1}{2}, 1\right\}, 0\right\}, 1 \right] \\
- \text{QL} \left[ \left\{\{1, 1, 1\}, \left\{\frac{1}{2}, 1\right\}, 0\right\}, z \right] + 2 \text{QL} \left[ \{\{1, 1, 1\}, \{2, 1, 1\}, 0\}, 1 \right] \right].
\]

(2.16)

\[
\text{TransformQL} \left[ \{\{1, 1, 1\}, \{2, 1, 1\}, 0\}, \frac{1 - z}{1 + z}, z \right] \\
\Rightarrow \text{QL} \left[ \{\{2, 1, 1\}, 0\}, 1 \right] \left[ \text{QL} \left[ \{\{1, 1, 0\}, 0\}, 1 \right] - \text{QL} \left[ \{\{1, 1, 0\}, 0\}, z \right] \right] \\
- \text{QL} \left[ \{\{3, 1, 0\}, 0\}, 1 \right] + \text{QL} \left[ \{\{3, 1, 0\}, 0\}, z \right] - \text{QL} \left[ \{\{3, 1, 0\}, 1\}, 1 \right] \\
+ \text{QL} \left[ \{\{3, 1, 0\}, 0\}, \{\{2, 1, 1\}, 0\}, 1 \right] \\
+ \text{QL} \left[ \{\{3, 1, 0\}, 0\}, \{\{2, 1, 1\}, 0\}, z \right] + \text{QL} \left[ \{\{3, 1, 0\}, 1\}, \{\{2, 1, 1\}, 0\}, 1 \right] \\
- \text{QL} \left[ \{\{3, 1, 0\}, 1\}, \{\{2, 1, 1\}, 0\}, z \right].
\]

(2.17)

In these transformations new special numbers are occurring beyond the multiple zeta values. In particular one obtains the values

\[
\text{QL} \left[ \{\{3, 0, 1\}, 1\}, 1 \right] = \ln(2) - \frac{1}{2} \ln(3)
\]

(2.18)

\[
\text{QL} \left[ \left\{\left\{\frac{1}{2}, 1\right\}, 0\right\}, 1 \right] = \frac{4}{\sqrt{7}} \arctan \left( \frac{\sqrt{7}}{3} \right)
\]

(2.19)
\[ \frac{2}{\sqrt{7}} \arctan \left( \frac{\sqrt{7}}{5} \right). \]  

(2.20)

More involved constants are dilogarithms of arguments, e.g., of the type \( \sqrt{3}(1 + i\sqrt{3})/(\sqrt{7} + \sqrt{3}) \), etc. and further special constants.

It is furthermore useful to transform \( QL \)-functions in a representation in which they have a convergent Taylor series representation, which is also applied in their numerical evaluation. This is provided by the command \texttt{QLToConvergentRegion}. An example is

\[
\text{QLToConvergentRegion}[\text{QL}[[\{1, 1, 1\}, 0], \{-1, 1, 0\}, \{2, 1, 1\}, 1], 4]]
\]

\[
= \text{QL}[[\{0, 1, 0\}, 0], 3] \text{QL}[[\{1, 1, 0\}, 0], 1] \text{QL}[[\{2, 1, 1\}, 1], 1] + \text{QL}[[\{2, 1, 1\}, 1], 1]
\]

\[
- \text{QL}[[\{2, 1, 0\}, 0], \{4, 1, 0\}, 0], 1] + \text{QL}[[\{1, 1, 0\}, 0], 1] - \text{QL}[[\{2, 1, 0\}, 0], 1]
\]

\[
\times \left( \frac{1}{2} \text{QL} \left[ \left[ \{0, 1, 0\}, 0, \left\{ \left\{ \frac{1}{2}, 1 \right\}, 0 \right\} \right], 1 \right] + \text{QL} \left[ \left[ \{0, 1, 0\}, 0, \left\{ \left\{ \frac{3}{2}, 1 \right\}, 1 \right\} \right], 1 \right] 
\]

\[
- \text{QL}[[\{2, 1, 1\}, 1], \{-1, 1, 0\}, 0], 1]] + \frac{1}{2} \text{QL} \left[ \left[ \left\{ \frac{3}{2}, 1 \right\}, 0 \right\}, 1 \right]
\]

\[
\times \text{QL} \left[ \left[ \left\{ \frac{3}{2}, 1 \right\}, 1 \right\}, 1 \right] + \text{QL}[[\{1, 1, 0\}, 0], \{-1, 1, 0\}, 0, \{2, 1, 1\}, 1], 1]
\]

\[
+ \frac{1}{2} \text{QL} \left[ \left[ \{1, 1, 0\}, 0, \left\{ \left\{ \frac{1}{2}, 1 \right\}, 0 \right\} \right], 1 \right]
\]

\[
+ \text{QL} \left[ \left[ \{1, 1, 0\}, 0, \left\{ \left\{ \frac{3}{2}, 1 \right\}, 1 \right\} \right], 1 \right]
\]

\[
+ 3 \text{QL}[[\{4, 1, 0\}, 0], \{2, 1, 0\}, \{14, 7, 1\}, 0], 1]
\]

\[
+ \text{QL}[[\{4, 1, 0\}, 0], \{2, 1, 0\}, \{14, 7, 1\}, 1], 1].
\]  

(2.21)

For removing poles in the integration domain we rely on the formula

\[
H_{a_1, a_2, \ldots, a_n}(z) = \sum_{i=0}^{m} H_{b_1, b_2, \ldots, b_i}(z - p) H_{a_{i+1}, a_{i+2}, \ldots, a_n}(p)
\]  

(2.22)

where \( f_{b_i}(x) := f_{a_i}(x + p) \).

The following example illustrates the use of this formula to remove poles. Consider \( H_{((0,1,0),0),((1,-1,0),0),((1,0,1),0)}(z) \). It has a pole at 1 due to the letter

\[
\frac{1}{-1 + x} = ((-1, 1, 0), 0).
\]  

(2.23)

In order to remove this pole we use (2.22) which yields

\[
H_{((0,1,0),0),((1,-1,0),0),((1,0,1),0)}(z) = H_{((0,1,0),0),((1,-1,0),0),((1,0,1),0)}(1) + H_{((1,1,0),0),((1,0,1),0)}(z - 1) H_{((0,1,0),0),((1,0,1),0)}(1)
\]

\[
+ H_{((1,1,0),0),((0,1,0),0)}(z - 1) H_{((0,1,0),0),((1,0,1),0)}(1) + H_{((1,1,0),0),((0,1,0),0),((2,2,1),0)}(z - 1)
\]

Remove trailing zeros, i.e., the letter \((0, 1, 0), 0\) from the functions with argument \( x - 1 \), yields
Here the regularization is performed in adding

\[ H_{((1,0),0),((1,0),0),((1,0),0)}(1) + H_{((1,0),0),((1,0),0)}(z - 1)H_{((1,0),0),((1,0),0)}(1) \]

\[ + [H_{((1,0),0),((1,0),0)}(z - 1)H_{((1,0),0),((1,0),0)}(z - 1) - H_{((1,0),0),((1,0),0)}(z - 1)]H_{((1,1,0,0),((1,0),0),(1,1,0,0)}(1) + H_{((1,0),0),((1,0),0),(2,2,1,0)}(z - 1). \]

Now we replace

\[ H_{((1,0),0),((1,0),0)}(z - 1) = H_{((1,0),0),((1,0),0)}(\frac{z - 1}{p}) - H_{((1,0),0),((1,0),0)}(1) + v \cdot i\pi \]

(2.24)

and finally we remove leading ones, i.e., the letter \((-1, 1, 0, 0)\), which results in

\[
H_{((1,0),0),((1,0),0),((1,0),0),((1,0),0,0)}(x) = H_{((1,0),0),((1,0),0),((1,0),0),((1,0),0,0)}(x) - H_{((1,0),0),((1,0),0),((1,0),0,0)}(1) - H_{((1,0),0),((1,0),0,0)}(1) + H_{((1,0),0),((1,0),0,(2,2,1,0),0)}(z - 1) + v \cdot i\pi H_{((1,0),0),((1,0),0),(1,1,0,0)}(1)H_{((1,0),0),((1,0),0)}(z - 1),
\]

where we set

\[
v = \begin{cases} 
1, & \text{for adding } +ie \text{ to a singular letter} \\
0, & \text{to compute Chauchy’s principal value} \\
-1, & \text{for adding } -ie \text{ to a singular letter}.
\end{cases}
\]

(2.25)

Note that it might be necessary to perform the above steps several times to different poles.

The series expansion of a QL-function \( H_m(z) \) with a letter

\[
\frac{1}{x + a_i}
\]

(2.26)

for \( a_i \in \mathbb{R}\setminus\{0\} \) is convergent for \( |z| < |a_i| \). Hence given a QL-function \( H_m(z) \) with letters from \( \mathcal{L}_{KP} \), i.e., with letters of the form (2.26), we remove all poles \( p \) at the real axis for

\[
\int_0^1 dx \int_0^x dy \frac{1}{[\frac{3}{8} - x]} \frac{1}{[\frac{15}{8} - y]} \rightarrow \lim_{\epsilon \to 0^+} \int_0^1 dx \int_0^x dy \frac{1}{[\frac{3}{8} - x - i\epsilon]} \frac{1}{[\frac{15}{8} - y]} \]

\[
= -\zeta_2 + 4 \ln^2(2) + 2 \ln(2) \ln(3) + \ln^2(3) - \ln^2(5) - [2 \ln(2) + \ln(3) - \ln(5)] \ln(7)
\]

\[
+ Li_2\left(-\frac{1}{4}\right) + Li_2\left(\frac{7}{12}\right) + i\pi [2 \ln(2) - \ln(5)]
\]

\[
= \text{QLEval} \left[ \{ \{ \frac{3}{8}, -1, 0 \}, 0 \}, \{ \{ \frac{15}{8}, -1, 0 \}, 0 \} \right], 1, 25, \text{PrincipalValue} \rightarrow \text{False}
\]

\[
\approx -0.8205920210842043836307006 - 0.70102614150465864209879799i.
\]

(2.28)

Here the regularization is performed in adding \( +ie \) to the denominator of the singular letters.

The QL-functions in the variable \( z \in [0, 1] \) can be Mellin transformed by

\[
M[f(x)](N) = \int_0^1 dx x^N f(x).
\]

(2.29)
One obtains representations by harmonic sums [3,4] and (generalized) S-sums [7] at complex weights

\[ S_{b,d}(N) = \sum_{k=1}^{N} \frac{(\text{sign}(b))^k}{k^{|b|}} S_{\phi}(k), \quad S_{\phi} = 1, b, \quad a_i \in \mathbb{Z} \setminus \{0\} \] (2.30)

\[ S_{b,d}(c, \bar{d}, N) = \sum_{k=1}^{N} \frac{b^c}{k^d} S_{\phi}(\bar{a}, k), \quad S_{\phi} = 1, \quad b, a_i \in \mathbb{C}, \quad c, d_i \in \mathbb{N} \setminus \{0\}. \] (2.31)

Instead of working with differential equations one may work with difference equations, which are solved by the package SIGMA [22,23]. The ground field of the package needs then to contain the corresponding special constants arising in \{c_i\}.

An example is the Mellin transformation of

\[ F_1(x) = \mathcal{M}[\mathcal{L} \left\{ \left\{ \{0,1,0\},0 \right\}, \left\{ \left\{ \frac{1}{3},0,1 \right\},1 \right\}, \left\{ \left\{ \frac{1}{3},0,1 \right\},1 \right\} \right\}, x], \] (2.32)

which is given by

\[
\mathbf{M}[F_1(x)](N) = -\frac{1}{(1+N)^3} - \frac{9T_1^2}{2(1+N)^3} + \frac{9T_3}{2(1+N)^3} + \frac{9T_4}{1+N} + T_4 \left( \frac{3}{(1+N)^3} + \frac{9T_2}{1+N} \right)
\]

\[
+ \left[ \frac{3T_5}{2(1+N)^3} + T_6 \left( \frac{1}{2(1+N)^3} - \frac{3T_1}{2(1+N)^3} + \frac{S_1}{4(1+N)^2} - \frac{S_1}{2(1+N)^2} \right) \right] iN
\]

\[
+ \frac{3iT_5^2 \sqrt{3}}{4(1+N)^2} \frac{i}{\sqrt{3}} \left[ S_{1,1}(1,-i\sqrt{3}) + S_{1,1}(1,1-i\sqrt{3}) - S_{1,1}(1,1+i\sqrt{3}) \right] iN
\]

\[
+ \left[ \frac{3T_5}{2(1+N)^3} + T_6 \left( \frac{1}{2(1+N)^3} - \frac{3T_1}{2(1+N)^3} + \frac{S_1}{4(1+N)^2} - \frac{S_1}{2(1+N)^2} \right) \right] i\frac{i}{N}
\]

\[
- \frac{3iT_5^2 \sqrt{3}}{4(1+N)^2} \frac{i}{\sqrt{3}} \left[ S_{1,1}(1,i\sqrt{3}) + S_{1,1}(1,1-i\sqrt{3}) - S_{1,1}(1,1+i\sqrt{3}) \right] iN
\]

\[ \times i^N \right) 3^{-N/2}. \] (2.33)

where we dropped the argument \( N \) both for the harmonic and generalized harmonic sums. The constants \( T_i \) are iterated integrals at \( x = 1 \) and are given by

\[ T_0 = \frac{\pi}{3\sqrt{3}} \] (2.34)

\[ T_1 = \frac{\ln(2)}{3} \] (2.35)

\[ T_2 = \frac{\zeta_2}{12} + \frac{\ln^2(3)}{24} + \frac{1}{12} \text{Li}_3\left(-\frac{1}{3}\right) \] (2.36)

\[ T_3 = \frac{1}{72} \zeta_3 - \frac{1}{27} \ln^3(2) + \frac{1}{36} \ln^2(2) \ln(3) \]

\[ - \frac{1}{36} \ln^2(2) \text{Li}_2\left(\frac{1}{4}\right) - \frac{1}{72} \text{Li}_3\left(\frac{1}{4}\right) \] (2.37)

\[ T_4 = \frac{1}{36} \zeta_2 \ln(2) - \frac{1}{36} \zeta_3 + \frac{1}{54} \ln^3(2) \]

\[ + \frac{1}{53} \ln(2) \text{Li}_2\left(\frac{1}{4}\right) + \frac{1}{36} \text{Li}_3\left(\frac{1}{4}\right) \] (2.38)

\[ T_5 = -\frac{1}{6\sqrt{3}} \text{Re}\left[ i\text{Li}_2\left(\frac{1}{2} + i\frac{\sqrt{3}}{2}\right) \right] \]

\[ = 2\zeta_2 - \frac{86}{33} \ln^2(3) + \frac{5}{33} \text{Li}_2\left(-\frac{1}{3}\right), \] (2.39)

where \( \text{Li}_n(x) \) denotes the classical polylogarithm [24] with the representation

\[ \text{Li}_n(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^n}, \quad x \in [-1, 1], \quad n \in \mathbb{N}. \] (2.40)
Not all of the above polylogarithms are independent, cf. [25,26], and the following relations hold,

\[ \text{Li}_2\left(\frac{1}{4}\right) = -\text{Li}_2\left(-\frac{1}{3}\right) - 2 \ln^2(2) + 2 \ln(2) \ln(3) - \frac{1}{2} \ln^2(3) \]

(2.41)

\[ = 2\text{Li}_2\left(-\frac{1}{2}\right) + \zeta_2 - \ln^2(2) \]

(2.42)

\[ \text{Li}_3\left(\frac{1}{4}\right) = \frac{7}{2} \zeta_3 - 2 \zeta_2 \ln(2) + \frac{2}{3} \ln^3(2) + 4\text{Li}_3\left(-\frac{1}{2}\right). \]

(2.43)

The basis of contributing constants is here

\[ \left\{ \ln(2), \zeta_2, \zeta_3, \pi, \ln(3), \text{Li}_2\left(-\frac{1}{2}\right), \text{Li}_3\left(-\frac{1}{2}\right) \right\}. \]

(2.44)

The constants at position 1–3 are multiple zeta values [2], at position 4 and 5 they are cyclotomic [9], and the ones at position 6 and 7 occurred already for square-root valued iterated integrals [26]. The Mellin transformation (2.33) is real.

### III. PHYSICS EXAMPLES

As an application of the operations given in Sec. II we calculate a few examples of particular iterated integrals, which have emerged in the calculation of inclusive Compton scattering cross sections at next-to-leading order (NLO) [16] recently. The corresponding integrals were defined by

\[ G_{b,\bar{a}}(x) = \int_0^x dw_b(x')G_{\bar{a}}(x'), \]

(3.1)

with

\[ dw_b(x) = \frac{ydx}{x}, \quad dw_{\bar{a}}(x) = \frac{dx}{x-a}, \quad a \in \mathbb{R}, \]

(3.2)

where \( y = \sqrt{x/(4+x)} \), \( x = s/m^2 - 1 \), \( s \) the cms energy and \( m \) a mass, implying \( y \in [0,1] \), and \( y = y(x) \).

Iterative integrals obey shuffle algebras [27–29] and are first reduced to a corresponding basis representation by exploiting the relations implied by (2.7). The formal iterated integrals (3.1) are given by

\[
G_{0,y,-1}(x), \quad G_{y,-1,0}(x), \quad G_{y,0,-1}(x), \quad G_{y,-1,-1}(x), \\
G_{y,-2,-1}(x), \quad G_{-4,y,-1}(x), \quad G_{y,-1}(x), \quad G_{y,y,-1}(x),
\]

(3.3)

and \( x = 4y^2/(1-y^2) \).

We now cast these integrals into a root–free form. Furthermore, we choose a simple main argument, to allow further iterated integration, needed in potential higher order calculations. For the following representations we choose the variable

\[ z = \frac{1-y}{1+y} \]

(3.4)

for the main argument and set \( H_2(z) \equiv H_2 \) for the harmonic polylogarithms and cyclotomic harmonic polylogarithms.

We now transform the integrals (3.3) into iterative integrals, see also [20,21], containing also letters generated by quadratic forms.

\[
G_{0,y,-1}(x) = -\frac{4}{3} \zeta_3 - \frac{1}{6} H_3 + \frac{2}{3} \zeta_2 H_1 + H_0^2 H_1 \\
- \sqrt{3} \pi H_{(3;0),0}(1) - 2H_{0,0,1} - 2H_{0,0,6,6} \\
+ 2H_{0,0,6,6} - 2H_1_{0,0,6,6} + 4H_{1,0,6,1} \\
+ \frac{4z}{(1-z^2)^2}(H_{-1}(x) + H_{1}(6)) - 2H_{1,6,1}) \\
+ \left[ \frac{4z}{(1-z^2)^2} + \frac{2}{3} \zeta_2 + 2H_{0,1} \right] H_0.
\]

(3.5)

Some of the iterated integrals in the right-hand side (rhs in (3.5) are obtained at main argument \( x \), like \( H_{-1}(x) \) and \( H_{0,-1}(x) \). It appears to be useful to use the following relations

\[ H_{-1}(x) = -H_0 - H_{1,6,1} + 2H_{1,6,1}. \]

(3.6)

\[ H_{-2,-1}(x) = \frac{1}{2} H_0^2 + H_{0,6,0} - 2H_{0,6,1} - 2H_{1,6,1} \\
- 2H_{1,6,1} - 4H_{1,6,1} + \frac{1}{2} \zeta_2 \]

(3.7)

\[ H_{0,-1}(x) = \zeta_2 + \frac{1}{2} H_0^2 + 2H_0 H_1 - 2H_{0,1} + H_{0,6,0} \\
- 2H_0_{6,6} + 2H_{1,6,0} - 4H_{1,6,1}. \]

(3.8)

which yields

\[
G_{0,y,-1}(x) = -\frac{4}{3} \zeta_3 - \frac{1}{6} H_3 + \frac{2}{3} \zeta_2 H_1 + H_0^2 H_1 \\
- \sqrt{3} \pi H_{(3;0),0}(1) - 2H_{0,0,1} - 2H_{0,0,6,6} \\
+ 2H_{0,0,6,6} - 2H_1_{0,0,6,6} + 4H_{1,0,6,1} \\
+ \left[ \frac{1}{3} \zeta_2 + 2H_{0,1} \right] H_0.
\]

(3.9)
For the other integrals the following results are obtained,

\[ G_{y,-1,0}(x) = \frac{2}{3} \zeta_3 + \zeta_2 H_0 - \frac{1}{6} H_0^3 - 2H_{0,0,1} - H_{0,[6],0} - 2H_{0,[6],1} + 2H_{0,[6],1} + 4H_{0,[6],1} \tag{3.10} \]

\[ G_{y,0,-1}(x) = \frac{2}{3} \zeta_3 - \zeta_2 H_0 - \frac{1}{6} H_0^3 - 2H_{0,0,1} + \sqrt{\pi} H_{[3],0}(1) + 4H_{0,0,1} - H_{0,[6],0} + 2H_{0,[6],1} - 2H_{0,[6],1} + 4H_{0,[6],1} \tag{3.11} \]

\[ G_{y,-1,-1}(x) = \frac{5}{9} \zeta_3 - \frac{1}{6} H_0^3 + \frac{\pi}{\sqrt{3}} H_{[3],0}(1) - H_{0,0,[6]} + 2H_{0,0,[6]} - H_{0,[6],0} - 4H_{0,[6],1} + 2H_{0,[6],1} + 2H_{0,[6],1} - 4H_{0,[6],1} \tag{3.12} \]

\[ G_{y,-2,-1}(x) = \frac{1}{12} \zeta_3 + \frac{1}{2} \zeta_2 H_0 - \frac{1}{6} H_0^3 - \frac{1}{4} \sqrt{3} \pi H_{[3],0}(1) - H_{0,0,[6]} + 2H_{0,0,[6]} + 2H_{0,[4],1} + 2H_{0,[4],1} - 2H_{0,[6],1} \tag{3.13} \]

\[ G_{y,-4,-1}(x) = \frac{16}{9} \zeta_3 - \frac{1}{6} H_0^3 + H_{-1}\left(-\frac{2}{3} \zeta_2 + H_0\right) + H_{0}\left(\frac{1}{2} \zeta_2 - 2H_{-1}\right) + \frac{2\pi}{\sqrt{3}} H_{[3],0}(1) \]

\[ + 2H_{-1,0,[6]} - 4H_{-1,0,[6]} + 2H_{0,0,-1} - H_{0,0,[6]} + 2H_{0,0,[6]} \tag{3.14} \]

\[ G_{y,-1}(x) = -\frac{1}{3} \zeta_2 + \frac{1}{2} H_0^2 + H_{0,[6]} - 2H_{0,[6]} \tag{3.15} \]

\[ G_{y,0,-1}(x) = \frac{2}{3} \zeta_3 + \frac{1}{3} \zeta_2 H_0 - \frac{1}{6} H_0^3 - H_{0,0,[6]} + 2H_{0,0,[6]} \tag{3.16} \]

where

\[ H_{[3],0}(1) = -\frac{2}{\sqrt{3}} \text{Cl}_2\left(\frac{2}{3} \pi\right) = \frac{2}{9} \left[ 4 \zeta_2 - \psi'(\frac{1}{3}) \right] \tag{3.17} \]

is another cyclotomic constant and \( \text{Cl}_2 \) denotes a Clausen functions with

\[ \text{Cl}_2(x) = \sum_{k=1}^{\infty} \frac{\sin(kx)}{k^2} \tag{3.18} \]

and \( \psi' \) denotes the first derivative of the digamma function.

The above functions contain letters of the usual harmonic polylogarithms and those of cyclotomy \( c = 3, 4 \) and 6 [9], to which the notation in (3.9)–(3.16) corresponds. This is the case because of the choice of the variable \( x \), which is possible in the univariate case, although one does not know the optimal choice \( a \text{ priori} \). The cyclotomic letters are characterized by two indices [9] as, e.g.,

\[ f_{[3]}(x) = \frac{x^3}{1 + x + x^2 + x^3 + x^4} \tag{3.19} \]

where the second index is smaller than the degree of the denominator polynomial.

Choosing the variable \( y \) instead as the main argument, one transforms the above expressions using Eq. (2.17). As a consequence the additional letters

\[ \left\{ \frac{1}{1 + 3x^2}, \frac{x}{1 + 3x^2} \right\} \tag{3.20} \]

are needed, which are not cyclotomic. As an example one obtains
we consider a real extension of the Kummer integrals, and also iterated integrals over square roots of numbers occur in this context. Often particular algebraic numbers may be present. Generally also $QL$-functions at argument $z = 1$ will appear, inducing new constants. This set can be reduced to the algebraic basis by shuffle and stuffle relations [29]. Depending on the defining constants of the contributing quadratic forms, further sets of relations may be present.

**IV. CONCLUSIONS**

In the analytic calculation of Feynman diagrams hierarchies of function spaces and algebras emerge both in the $z$ space and $N$ space representation consisting out of iterative integrals or nested sums of different kind. The simplest structures are harmonic polylogarithms, followed by Kummer–Poincaré iterated integrals and cyclotomic integrals, and also iterated integrals over square–root valued letters and the associated sums and special constants. Here we consider a real extension of the Kummer–Poincaré iterated integrals, allowing also for letters generated by general real quadratic forms without real factorization. Here the range of constants is not limited to $c_i \in \mathbb{Q}$, but general real numbers are allowed, which are usually implied by the values of different masses and virtualities in the processes to be considered. Quantities of this kind appear in higher order and multileg calculations. Since real representations have sometimes advantages compared to complex representations, we provide algorithms to build the associated algebra to a set of these letters, their basis representation, different mappings of the main argument, including analytic continuation in the case of the presence of cuts. Finally, also the expressions can be evaluated numerically. The different commands in HarmonicSums to provide these operations are described and illustrated by examples. We have applied the corresponding mappings to a class of functions which have emerged recently in the NLO calculation of the inclusive Compton cross section. In viewing physics results within this class, it is for structural reasons also interesting to see whether the result can be expressed by functions out of a particular function space. In the case of Ref. [16] it turns out to be the space of cyclotomic harmonic polylogarithms if the final expression is written using the variable $z$, (3.4).

The different commands to treat iterated integrals of the $QL$-type are implemented in the package HarmonicSums, which is available from https://risc.jku.at/sw/harmonicsums/. As well we attach the Supplemental Material Quadratic-Letters.nb to this paper [30].

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