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The q-extension of iterated integrals and nested sums in quantum field theory

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Abstract

Analytic calculations of zero- and single-scale quantities in perturbative quantum field theory result into special numbers and functions, the first of which have been revealed during the last decades. These are generalizations of the polylogarithm in form of Kummer-Poincaré iterative integrals over special alphabets and extensions thereof. With growing order in the coupling constant, the polylogarithms, Nielsen integrals, the iterated integrals over linear denominator terms, cyclotomic letters, letters induced by quadratic forms, square-root valued letters, and more general functions contribute. For the nested sums we consider nested harmonic sums, generalized harmonic sums, nested sums implied by quadratic forms, cyclotomic harmonic sums, and nested sums containing central binomials. We construct the q-extensions of these special functions and of the nested sums, which are associated to them by the series expansion at $x = 0$, and their Mellin transform in the q-free case. These functions are expected to play a role in perturbative calculations in the case of q-deformed commutation relations. For the simpler function spaces closed form solutions are presented. For more involved alphabets we present the algorithmic steps leading to the q-extension for the individual cases. We also derive the determining differential and difference equations of these higher transcendental functions. The q-extended special functions are quite different form the corresponding μ-extended functions.

1 Introduction

The q-extension of mathematical functions, i.e. the association of the so-called basic-function to a given function, has a very long history, see Ref. [1]. q-analogues have been calculated for many special functions, as described in the surveys Refs. [2–17]. In particular, the q-extension of the generalized hypergeometric functions and their generalizations, like the Appell-functions, Lauricella-functions and others, Ref. [4–6,18,19], play a central role, cf. Refs. [20–22], since these functions cover large classes of special functions. It applies to different type orthgonal polynomials [9, 10].[1] Also the Bessel functions belong to the class of hypergeometric solutions, which are extended to the Jackson q-Bessel and Hankel functions [7,37,61–68]. The Al-Salam-Chihara polynomials are closely related to representations of the quantized universal enveloping algebra $U_q(su(1,1))$. The Hall-Littlewood symmetric functions [53], with extension to the multivariate Rogers-Szegö polynomials H_n and generalized Galois numbers, are linked to affine Kac-Moody algebras [69]. Many of the q-orthogonal polynomials occupy distinguished positions within the Askey scheme [10, 70] and play a central role in harmonic analysis [71] and algebraic combinatorics.

The q-extensions are applied to quantum mechanical systems modifying the Heisenberg algebra by the q-deformation [72, 73]

$$\hat{x}\hat{p} - q\hat{p}\hat{x} = i, \tag{1.1}$$

where q denotes the parameter of the extension, and $\hat{x}$ and $\hat{p}$ are the position and the momentum operators.

Within this framework, q-analogues in quantum mechanics, such as for the Schrödinger equation, conformal quantum mechanics, and harmonic oscillator systems were constructed and analyzed [74–79], as well as Lie algebra representations were given in Refs. [80–84]. Extensions were made to p,q-deformed oscillators [85–88] linked to the quantum algebra $su(2)_{p,q}$ and a large number of versions of q-oscillators were considered [89–93], as contained in the p,q-family of deformed oscillators. Furthermore, 3-, 4-, and even 5-parametric deformed oscillators proposed in [94–96] were studied and so-called k-bonacci [97] or quasi-Fibonacci [98] structures were found. Deformed Heisenberg algebras were investigated in Refs. [93,99–101]. Also, it is worth to emphasize that deformed oscillator algebras are naturally considered as the respective modified 'boson' algebras, cf. Refs. [102–105].

Quantum mechanical q-extensions were also used for the thermostatistical description of q-bosons in Refs. [106–114]. Another important application is the use of q-analogues for the description of hadron flavor symmetries in Refs. [115–118] based on such q-deformed structures as quantum groups $SU_q(N_F)$ and quantum algebras $U_q(su_N)$ in Refs. [115, 117–126]. In these analyses new hadron mass sum rules were obtained at high precision [115,118,121–128]. In several applications [129, 130] the Lerch transcendent $\Phi(z,\alpha,\beta)$, Ref. [131], which covers a wide set of functions, occurs. In Ref. [113] (p,q)-extended polylogarithms and the associated ζ-function emerge. Bi-basic hypergeometric functions [7] occured in Ref. [98]. In supersymmetric extensions [132,133] twin-basic hypergeometric functions [7] emerge. The q-Gegenbauer polynomials [27] are

[1] It concerns the q-extensions of the Al-Salam-Chihara polynomials [23], Jacobi polynomials [24–29], Legendre polynomials [30–33], Gegenbauer polynomials [34–36], Laguerre polynomials [37], Koornwinder polynomials [38], Hermite polynomials [39,40], Lommel polynomials [41,42], Krawtchouk polynomials [43–45], Chebyshev polynomials [46], Meixner polynomials [47], Charlier polynomials [48], Wilson polynomials [49], Hahn polynomials [20], the q-binomial polynomials, called Rogers-Szegö polynomials [50–52], and Hall-Littlewood symmetric functions [53], the q-binomial coefficient or Gaussian polynomial with extension to q-multinomial coefficients [54, 55], the q-disk polynomials [56, 57], and the Macdonald polynomials, related to the one-row Young diagrams [58–60].

applied in the q-extension of spin-network approaches [134]. In meson mass sum rules [115,122], certain q-polynomials, such as the q-Chebyshev polynomials [46], emerge.

The q-extension in quantum field theories are implied by the modified commutation (or anti-commutation) relations

$$a_\lambda(k)a^\dagger_{\lambda'}(k') - qa^\dagger_{\lambda'}(k')a_\lambda(k) = g_{\lambda\lambda'}\delta^{(3)}(k-k'), \tag{1.2}$$

as shown in Ref. [135,136]. Here $a_\lambda(k)$ and $a^\dagger_{\lambda'}(k')$ are the creation and annihilation operators. The q-modified quantum field theories are related to approaches based on non-commutative space time [137–140] and quantum groups [141–145]. In the study of quantum groups, conformal field theory, and of integrable systems, the theory of the q-Virasoro algebra plays an important role, cf. Refs. [146–148]. Also q-supersymmetric theories and q-superalgebras have been studied, cf. Refs. [132,149–153].

The scope of the present paper is to construct the q-extensions of the different spaces of special functions occurring in perturbative calculations in quantum field theories of scattering processes to higher loop order in the non-modified case. These are classes of iterated integrals, such as polylogarithms [154–160], Nielsen integrals [161,162], followed by the harmonic polylogarithms [163]. They are special sub-spaces of the generalized harmonic polylogarithms, which were first introduced by E. Kummer, see Refs. [164–172]. Other extensions are the cyclotomic harmonic polylogarithms [173] and iterated integrals inspired by general quadratic forms [174]. In these classes the denominator functions are either linear functions or polynomials. There is a further class of functions obeying first order factorizing differential equations, based on alphabets containing square-root valued letters [175].

The series expansion of these functions around $x = 0$ or their Mellin transform lead to different classes of nested sums. These are the harmonic sums [176,177], the generalized harmonic sums [171, 172], and sums, which additionally contain central binomial factors [175]. These quantities have been reviewed in detail in Ref. [178]. In this paper we will derive their q-extension. In a preceding paper [178] we have studied the so-called μ-extension, see Refs. [179, 180] of the mentioned classes of generalized special functions. These extensions are, however, structurally very different from the q-extensions.

Like in the case of the μ-extension, the starting point is the closed-form solution $f[n]$ for the respective function[2] is

$$F(x) = \sum_{n=0}^{\infty} f[n]x^n. \tag{1.3}$$

The functions $f[n]$ have a sum-product representation in terms of nested sums. This function must be known in closed form for all integers $n \in \mathbb{N}$. The q-extension of $F(x)$ is obtained from the q-extension of $f[n]$, $f[n;q]$,[3]

$$F(x;q) = \sum_{n=0}^{\infty} f[n;q]x^n. \tag{1.4}$$

For q-extended nested sums and iterated integrals a number of algorithms were created, like the extension of Zeilberger's algorithm [181, 182] in Refs. [183–190] and Refs. [191–195], as well as operator methods for q-identities [196–198].

[2] Also modifications of Eq. (1.3) may be considered, see Ref. [178], Eqs. (6,7). For sums starting at $n = 1$ we add $f[0] = 0$ symbolically for technical reasons in the calculations below.

[3] We also use the notation $\langle x^n\rangle F(x;q) = f[n;q], \quad n \geq 0$.

Compared to the μ-extension of the different function classes studied in Ref. [178], the q-extensions define new function spaces of higher transcendental functions. Already the simplest quantities are given by q-hypergeometric functions. The corresponding difference and differential equations grow with the weight of the extended quantities. The main characteristics defining the respective q-extensions are the recurrence relations for the quantities $f[n;q]$ and the q-differential and q-shift relations for $F[x;q]$. The q-extended nested sums are defined by their recurrence relation. If the recursion for $f[n;q]$ is known, a fast numerical evaluation of $F(x;q)$, Eq. (1.4), around $x = 0$ is possible. Series representations of $F(x;q)$ have a finite convergence radius. To obtain the q-extension around a different point x_0, a further series expansion of $F(x)$ must be performed, ensuring that the domains of convergence for neighboring series overlap. Because of its similarity to Frobenius' method [199], which is in wide use in quantum field-theoretic calculations, see, e.g., [200–202], we call this method *q-Frobenius method*.

The paper is organized as follows. In Section 2 we summarize basic definitions and operations used to construct the q-extensions. All nested sums and iterated integrals for which we are constructing the q-extension obey first order factorizing difference and differential equations. A summary on these quantities has been given by us in Ref. [178] previously. The nested sums and iterated integrals are built over special alphabets of letters, $\mathfrak{S}$ or $\mathfrak{A}$. The q-extensions of the different classes of nested sums are derived in Section 3 and the ones for the iterated integrals in Section 4. Here we also derive the defining equations. For the simple cases, such as the single harmonic sums, the polylogarithms and Nielsen integrals, one can derive general representations. For the more involved alphabets we device the sequence of algorithmic steps to obtain the result in each individual case. Like in the q-free case, only a finite amount of nested finite sums and iterated integrals contributes in perturbative field-theoretic calculations up to a certain power in the coupling constant. In Section 5 we discuss the shuffle algebras for the q-extended iterated integrals and the quasi-shuffle algebras for the q-extended nested sums. Their use allows one to significantly reduce the number of contributing terms at a given weight. Section 6 contains the conclusions.

2 Basic Definitions

We first summarize relations given in the literature for the asymmetric q-extension[4], which we use in the following, see Refs. [1–7, 9, 11–13]. The q-extension of an integer number n is given by

$$\{n\}_q = \frac{1-q^n}{1-q} = \sum_{k=0}^{n-1} q^k, \quad \text{with} \quad q \in [0,1]. \tag{2.1}$$

The variables n occurring in powers

$$c^n, \quad c \in \mathbb{C}, \tag{2.2}$$

are not q-extended.

The Jackson q-derivative is defined by [205–208]

$$\mathcal{D}_x^q f[x] = \frac{f(x) - f(qx)}{(1-q)x}, \tag{2.3}$$

[4]There are also other q-extensions, see Appendix A of Ref. [178]. The symmetric q-extension, which obeys the symmetry $q \leftrightarrow q^{-1}$ is applied in Refs. [77, 78, 144], two-variable extensions were used in Refs. [85, 86, 203], and multi-parameter extensions in Refs. [94–96, 99, 100, 204].

with

$$\mathcal{D}_x^q[x^\alpha] = \frac{(1-q^\alpha)}{(1-q)} x^{\alpha-1}, \quad \alpha \in \mathbb{R}, \tag{2.4}$$

for the power function. The operator $\mathcal{D}_x^q$ becomes only a differential operator in the limit $q \to 1^-$. Otherwise it is a difference operator, by which the q-differential (2.32) and q-shift relations (2.31), derived for the iterated integrals below, are related.

The q-extended Pochhammer symbol [209] reads, cf. Ref. [197],

$$(a;q)_n = \prod_{k=0}^{n-1}(1-aq^k), \quad (a;q)_0 = 1, \tag{2.5}$$

$$(q;q)_n = \prod_{k=1}^{n}(1-q^k), \quad (q^2;q)_n = \prod_{k=2}^{n+1}(1-q^k). \tag{2.6}$$

The *rising* Pochhammer symbol $(x)_n$ can be written in terms of the Stirling numbers of the 1st kind [210], respectively for their q-extension,

$$(x)_n = \sum_{k=0}^{n} s(n,k)(-1)^{n-k}x^k, \tag{2.7}$$

$$(x;q)_n = \sum_{k=0}^{n} s(n,k;q)(-1)^{n-k}x^k, \tag{2.8}$$

for which the recursions

$$\begin{aligned} s(n+1,k) &= s(n,k-1) - n\; s(n,k), \\ & \quad s(0,0) = 1, \quad s(n,0) = 0 \quad \text{for} \quad n > 0, \quad s(0,k) = 0 \quad \text{for} \quad k > 0, \end{aligned} \tag{2.9}$$

$$\begin{aligned} s(n+1,k;q) &= s(n,k-1;q) - \{n\}_q\; s(n,k;q), \\ & \quad s(0,0;q) = 1, \quad s(n,0;q) = 0 \quad \text{for} \quad n > 0, \quad s(0,k;q) = 0 \quad \text{for} \quad k > 0, \end{aligned} \tag{2.10}$$

hold.

The q-extended factorial, the Gaussian q- and central binomial [211] are given by

$$\{n!\}_q = \prod_{k=1}^{n}\{k\}_q = \Gamma_q(n+1), \tag{2.11}$$

$$\binom{n}{m}_q = \frac{(q)_n}{(q)_m(q)_{n-m}} = \prod_{i=0}^{m-1}\frac{1-q^{n-1}}{1-q^{i+1}}, \tag{2.12}$$

$$\binom{2n}{n}_q = \frac{\{2n!\}_q}{\{n!\}_q^2}. \tag{2.13}$$

Due to

$$\binom{n+1}{k}_q = q^k\binom{n}{k}_q + \binom{n}{k-1}_q, \quad \binom{n}{1}_q = \frac{1-q^n}{1-q}, \quad \binom{n}{2}_q = \frac{(1-q^n)(1-q^{n-1})}{(1-q)(1-q^2)} \tag{2.14}$$

the q-binomial is a polynomial, since the initial values are polynomials in q, because for each n $(1-q^n)$ contains the factor $(1-q)$ and for each even n the factor $(1-q^2)$.

For real argument z,

$$\Gamma(z+1) = z\Gamma(z), \quad z \notin \{\mathbb{Z}, z < 1\}, \tag{2.15}$$

the function Γ_q is defined by

$$\Gamma_q(z+1) = \frac{1-q^z}{1-q}\Gamma_q(z), \quad \Gamma_q(1) = 1. \tag{2.16}$$

Related to it, the digamma function is

$$\psi(z) = \frac{d}{dz}\ln[\Gamma(z)], \tag{2.17}$$

$$\psi(z+1) = \frac{1}{z} + \psi(z), \quad z \notin \{\mathbb{Z}, z < 1\}. \tag{2.18}$$

The functions $\psi_q^{(n)}, n \geq 0$, are given by

$$\psi_q(z) = \frac{d}{dz}\ln[\Gamma_q(z)] = -\ln(1-q) + \ln(q)\sum_{n=0}^{\infty}\frac{q^{n+z}}{1-q^{n+z}}, \tag{2.19}$$

$$\psi_q^{(n)}(z) = \frac{d^n}{dz^n}\psi_q(z). \tag{2.20}$$

The last sum in (2.19) is a modified Lambert series $\mathrm{L}(q)$, [212, 213],

$$\mathrm{L}(q) = \sum_{n=1}^{\infty}\frac{q^n}{1-q^n} = \frac{1}{\ln(q)}[\psi_q(1) + \ln(1-q)]. \tag{2.21}$$

The asymptotic expansion of $\psi_q(z)$ in the limit $z \to \infty$ is given by [214]

$$\psi_q(z) \propto \ln\left(\frac{1-q^z}{1-q}\right) + \frac{\ln(q)}{2(q^{-z}-1)} - \sum_{k=1}^{\infty}\frac{B_{2k}}{(2k)!}\left(\frac{\ln(q)}{(1-q)^z}\right)^{2k} q^z P_{2k-2}(q^z), \tag{2.22}$$

$$P_n(x) = x(1-x)\frac{d}{dx}P_{n-1}(x) + (nx+1)P_{n-1}(x), \quad P_0 = 1, \quad n \geq 1, \quad P_n(1) = (n+1)!, \tag{2.23}$$

with B_{2k} the usual Bernoulli numbers. The first polynomials are

$$P_1(x) = 1 + x, \tag{2.24}$$

$$P_2(x) = 1 + 4x + x^2, \tag{2.25}$$

$$P_3(x) = 1 + 11x + 11x^2 + x^3, \quad \text{etc.} \tag{2.26}$$

The q-polygamma functions $\psi_q^{(n)}(z)$ can be used to define the single q-harmonic sums, as the polygamma functions are also the analytic continuations of the single harmonic sums, cf. [177], after the proper treatment of factors of $(-1)^n$, in terms of a suitable Mellin transform, see Ref. [177] and Section 3.

Heine [2, 3] introduced the q-generalization of the hypergeometric series. The q-extended generalized hypergeometric series are given by

$${}_{s+1}\phi_s\left(\begin{matrix}a_1, a_2, \ldots, a_{s+1}\\ b_1, b_2, \ldots, b_s\end{matrix}; q, z\right) = \sum_{n=0}^{\infty}\frac{(a_1;q)_n(a_2;q)_n\cdots(a_{s+1};q)_n}{(q;q)_n(b_1;q)_n\cdots(b_s;q)_n}z^n. \tag{2.27}$$

The q-extended generalized hypergeometric series provide a flexible framework.[5] which can be used for some special cases in the following. These functions were studied in detail in Refs. [4–7, 11, 13, 216].

The q-differential equation of the q-hypergeometric function $u(x) = {}_2\phi_1$ is given by [216]

$$\left\{x(b_1 - a_1a_2qx)(\mathcal{D}_x^q)^2 + \left[\frac{1-b_1}{1-q} + \frac{(1-a_1)(1-a_2) - (1-a_1a_2q)}{1-q}\right]\mathcal{D}_x^q - \frac{(1-a_1)(1-a_2)}{(1-q)^2}\right\}$$
$$\times {}_2\phi_1\left(\begin{matrix}a_1, a_2\\ b_1\end{matrix}; q, u\right) = 0. \tag{2.28}$$

An equivalent representation is [216]

$$[b_1 - a_1a_2qx]u(q^2x) + [q(a_1a_2(q+1)(x-1) + a_1 + a_2 - 1) - b_1]u(qx)$$
$$-[q(x-1)(a_1(a_2q + a_2 - 1) - a_2 + 1]u(x) = 0, \tag{2.29}$$

which is also called q-shift relation.

For the q-extended nested sums we will derive difference equations

$$\sum_{k=0}^{M} s_k(n;q) f[n+k;q] = 0, \tag{2.30}$$

where $s_k(n;q)$ are polynomials of q-exponential terms q^{ln+m}.

The q-extended iterated integrals have three representations.

i) the recurrence of the q-extension of $f[n]$, $f[n;q]$, given by Eq. (2.30).

ii) the q-shift difference equation is given by

$$\sum_{k=0}^{M} r_k(x,q) F[xq^k] = 0, \tag{2.31}$$

where $r_k(x,q)$ are polynomials and for $F[xq^k]$ only the main argument is displayed, like in Eq. (2.29).

iii) the q-differential equation reads

$$\left[\sum_{k=0}^{M} p_k(x,q)(\mathcal{D}_x^q)^k\right] F[x;q] = 0. \tag{2.32}$$

All three relations can be transformed into each other. In the case of q-shift difference and q-differential equations one may use Eq. (2.3). In the limit $q \to 1^-$ one obtains the q-free case for all functions studied in the following.

3 The q-extensions of nested sums

We consider the alphabet

$$\mathfrak{S} = \{s_1(k), \ldots, s_m(k)\}, \quad k \in \mathbb{N}, \tag{3.1}$$

[5] They allow also to represent the elliptic polylogarithms, cf. Ref. [215].

where, $s_l(k)$ are sum-product structures. The nested finite sums are defined by

$$S_{a,b_1,\ldots,b_m}(N) = \sum_{k=1}^{N} s_a(k) S_{b_1,\ldots,b_m}(k), \tag{3.2}$$

where the letters a, b_i label elements out of $\mathfrak{S}$.

The following sum-types play a central role both for the representation of the Mellin transform Eq. (3.3) and in the analytic series expansion of the functions $f(x)$ around $x = 0$,

$$\mathbf{M}[f(x)](N) = \int_0^1 dx\ x^{N-1} f(x). \tag{3.3}$$

i) Harmonic sums.

The q-extension of the harmonic sums [176, 177] are given by

$$\begin{aligned} S_{b,\vec{a}}(n;q) &= \sum_{k=1}^{n} \frac{(\mathrm{sign}(b))^k}{\{k\}_q^{|b|}} S_{\vec{a}}(k;q), \quad S_\emptyset = 1, b, a_i \in \mathbb{Z}\backslash\{0\} & (3.4)\\ &= \sum_{k=1}^{n} (\mathrm{sign}(b))^k \left[\frac{1-q}{1-q^k}\right]^{|b|} S_{\vec{a}}(k;q). & (3.5) \end{aligned}$$

These sums contribute to the central functions $f[n;q]$ of the q-extended Nielsen integrals and the q-extended harmonic polylogarithms. In the limit $q \to 1^-$ the usual nested sums are obtained.

For the single harmonic sums one obtains

$$\begin{aligned} S_1(n;q) &= (1-q)\left\{n + \frac{1}{\ln(q)}\left[\psi_q(1) - \psi_q(n+1)\right]\right\}, & (3.6)\\ S_2(n;q) &= (1-q)^2\left\{n + \frac{1}{\ln(q)}\left[\psi_q(1) - \psi_q(n+1)\right] + \frac{1}{\ln^2(q)}\left[\psi_q^{(1)}(1) - \psi_q^{(1)}(n+1)\right]\right\}, & (3.7)\\ S_3(n;q) &= (1-q)^3\left\{n + \frac{1}{\ln(q)}\left[\psi_q(1) - \psi_q(n+1)\right] + \frac{3}{2\ln^2(q)}\left[\psi_q^{(1)}(1) - \psi_q^{(1)}(n+1)\right]\right. \\ &\quad \left. + \frac{1}{2\ln^3(q)}\left[\psi_q^{(2)}(1) - \psi_q^{(2)}(n+1)\right]\right\}, & (3.8) \end{aligned}$$

etc.

The recurrence for the single q-harmonic sums $S_l(N;q)$ is given by[6]

$$\begin{aligned} &-(1-q^{1+n})^l F[n;q] + \left[(1-q^{1+n})^l + (1-q^{2+n})^l\right] F[n+1;q] - (1-q^{2+n})^l F[n+2;q] = 0, \\ &F[1;q] = 1, \quad F[2;q] = 1 + \left(\frac{1-q}{1-q^2}\right)^l \end{aligned} \tag{3.9}$$

for $l \geq 1$. In the alternating case $l \leq -1$ one has

$$\begin{aligned} &-(1-q^{1+n})^l F[n;q] + \left[(1-q^{1+n})^l - (1-q^{2+n})^l\right] F[n+1;q] + (1-q^{2+n})^l F[n+2;q] = 0, \\ &F[1;q] = -1, \quad F[2;q] = -1 + \left(\frac{1-q}{1-q^2}\right)^l. \end{aligned} \tag{3.10}$$

[6]Here and in the following the recurrences are written in polynomial form for the coefficients, i.e. leaving out denominator factors like $(1-q)^l$ in (3.9) etc. They are valid for $q < 1$.

The recurrences for individual monomials can be obtained by using the command `GuessqRecurrence` from the package `qFunctions.m`, Ref. [217], or `QREGuess` from the package `qGeneratingFunctions.m`, Ref. [218, 219], or by direct construction of repeated use of Eq. (3.15) and similar relations. We had to apply different methods to find the recurrences derived in the following.[7] The number of expansion coefficients $f[n;q]$ for the expansions around $x = 0$ needed to determine the recurrences in the examples given below varies from $N = 15$ to 80, depending on the complexity of the problem. Related to this, the maximal order and degree in the search for the recurrences take values of up to $O(10)$. For the iterated integrals we used the procedures `QRE2DE` and `QRE2SE` [218] to find the q-differential and q-shift relations.

Examples for q-extended nested harmonic sums are

$$S_{2,1}(n;q) = \sum_{k=1}^{n} \left[\frac{1-q}{1-q^k}\right]^2 \sum_{l=1}^{k} \frac{1-q}{1-q^l}, \tag{3.11}$$

$$S_{3,-2}(n;q) = \sum_{k=1}^{n} \left[\frac{1-q}{1-q^k}\right]^3 \sum_{l=1}^{k} (-1)^l \left[\frac{1-q}{1-q^l}\right]^2. \tag{3.12}$$

The recurrence of $S_{2,1}(n;q)$ reads

$$\begin{aligned}
&\left(q^{n+1}-1\right)^2 \left(q^{n+2}-1\right) F[n;q] - \left(q^{n+2}-1\right) \left(-\left((q+1)(q+2)q^{n+1}\right) + \left(q^3+q^2+1\right) q^{2n+2}\right. \\
&\left.+3\right) F[n+1;q] + \left(q^{n+2}\left(-\left((q(3q+2)+4)q^{n+2}\right) + \left(q^3+q+1\right) q^{2n+4} + 4q + 5\right) - 3\right) \\
&\times F[n+2;q] - \left(q^{n+3}-1\right)^3 F[n+3;q] = 0,
\end{aligned} \tag{3.13}$$

and for $S_{3,-2}(n;q)$

$$\begin{aligned}
&\left(q^{n+1}-1\right)^3 \left(q^{n+2}-1\right)^2 F[n;q] + \left(q^{n+2}-1\right)^2 \\
&\times \left(\left(q\left(\left(3-(q-1)q^2(q+3)\right) q^n + \left(q^5-q^3-1\right) q^{2n+1} + 2q - 2\right) - 3\right) q^{n+1} + 1\right) F[n+1;q] \\
&+ \left(\left((q(11q+6)-7)q^{n+2} + (9 - q(q(10q+3)+6))q^{2n+4} + \left(q\left(5q^3+3q+2\right) - 5\right) q^{3n+6}\right.\right. \\
&\left.\left. - \left(q^5+q^2-1\right) q^{4n+8} - 7q + 2\right) q^{n+2} + 1\right) F[n+2;q] + \left(q^{n+3}-1\right)^5 F[n+3;q] = 0.
\end{aligned} \tag{3.14}$$

For the initial values of these recurrences, and analogously for those given below, we use the first values of the respective analytic expressions, like of Eqs. (3.11, 3.12).

For analytically known nested product-sum structures one can also construct the associate recurrence by systematic deconstruction using shift relations down to zero. As an example we consider the sum $S_{1,1}(n;q)$. By using

$$\frac{1-q^{n+1}}{1-q} \left[S_{1,1}(n+1;q) - S_{1,1}(n;q)\right] = S_1(n+1;q), \tag{3.15}$$

a reduction is obtained, which can be iterated until the r.h.s. vanishes. In this way one obtains the third-order linear homogeneous difference equation for $S_{1,1}(n;q)$,

$$\begin{aligned}
&\left(q^{n+1}-1\right) \left(q^{n+2}-1\right) S_{1,1}(n;q) - \left(q^{n+2}-1\right) \left(\left(q^2+q+1\right) q^{n+1} - 3\right) S_{1,1}(n+1;q) \\
&+ \left(\left(q^{n+2}-1\right)^2 + \left(q^{n+3}-1\right) \left(q^{n+2}-1\right) + \left(q^{n+3}-1\right)^2\right) S_{1,1}(n+2;q) \\
&- \left(q^{n+3}-1\right)^2 S_{1,1}(n+3;q) = 0.
\end{aligned} \tag{3.16}$$

[7] Other implementations are, e.g., `Gfun`, `HYPQ`, `RATE`, `QSERIES`, and `GUESS` [220–224].

The common recurrence of different sum-product monomials which obey q-holonomic sequences can be obtained by using closure properties, cf. Refs. [218, 225]. The command `QREPlus` [218] allows one to join two recurrences to a common one. We will use this procedure in some cases below.

ii) Generalized harmonic sums.
The q-extension of the generalized harmonic sums, cf. Refs. [171, 172] are given by

$$\begin{aligned} S_{b,\vec{a}}(\{c,\vec{d}\},n;q) &= \sum_{k=1}^{n} \frac{c^k}{\{k\}_q^b} S_{\vec{a}}(\vec{d},k;q), \quad S_\emptyset = 1, b, a_i \in \mathbb{N}\backslash\{0\}, c, d_i \in \mathbb{C}\backslash\{0\}, \\ &= \sum_{k=1}^{n} c^k \left[\frac{1-q}{1-q^k}\right]^b S_{\vec{a}}(\vec{d},k;q). \end{aligned} \tag{3.17}$$

These sums contribute to the central functions $f[n;q]$ of the q-generalized harmonic polylogarithms, the q-cyclotomic harmonic polylogarithms, and q-harmonic polylogarithms inspired by quadratic forms.

As an example we derive the recurrence for the generalized harmonic q-nested sum $S_{1,2}(-\frac{1}{2},2;n;q)$. It is obtained by

$$\begin{aligned} &\left(q^{n+1}-1\right)\left(q^{n+2}-1\right)^2 S_{1,2}(-\tfrac{1}{2},2;n;q) + \left(q^{n+2}-1\right)\Big(\Big(q\left(q\left(\left(q^3+2q-1\right)q^n-2\right)-3\right)+1\Big) \\ &\times q^{n+1}+2\Big) S_{1,2}(-\tfrac{1}{2},2;n+1;q) + \Big(\big(((2-5q)q+6)q^{n+2} + \left(q^2(2q-1)-2\right)q^{2n+4} + 4q \\ &-7\big)q^{n+2}+1\Big) S_{1,2}(-\tfrac{1}{2},2;n+2;q) - 2\left(q^{n+3}-1\right)^3 S_{1,2}(-\tfrac{1}{2},2;n+3;q) = 0. \end{aligned} \tag{3.18}$$

iii) Nested sums containing central binomials
In these sum-structures, which contain sums of the kind ii), additionally factors of

$$\left.\binom{2n}{n}\right|_q \tag{3.19}$$

are present, cf. Ref. [175]. An example will be dealt with in Section 4.7.

In summary, the q-extended nested finite sums obey q-difference equations of finite order and degree, which can be obtained by guessing methods, as, e.g., those of Ref. [217, 218]. Sums and products of these quantities form the expansion coefficients of the iterated integrals dealt with in Section 4. The quasi-shuffle properties of q-extended sums are discussed in Section 5.

4 The q-extended iterative integrals

The properties of the iterative integrals $F(x)$ for which we construct the q-extension in the following have been discussed in Section 3 of Ref. [178] already. By considering their series expansion at $x = 0$,

$$F(x) = \sum_{n=0}^{\infty} f[n] x^n, \tag{4.1}$$

the central function $f[n]$ is obtained which is needed to construct the q-extensions.[8] Here, all summation quantifiers and products are q-extended, while powers c^n, $c \in \mathbb{C}$ are not. The q-free

[8] For deriving relations for functions in the q-free case we apply algorithms of `HarmonicSums.m`, Refs. [226,227], see also Ref. [178].

functions are obtained in the limit $q \to 1^-$. In some cases the l'Hospital rule [228] has to be applied.

The q-extensions of all iterative integrals are higher transcendental functions. Some of them can be expressed as special q-extended (generalized) hypergeometric functions. As has been outlined in Ref. [178], this is different in the case of the μ-extension. There the class of special functions is preserved, except for the case of alphabets containing square-root valued letters.

One can derive closed form solutions for the q-extension of classical polylogarithms and Nielsen integrals. For higher classes of iterated integrals, because of a large amount of permutations of letters of the contributing alphabets $\mathfrak{A}$, we will devise methods to derive the q-extension for the respective cases. Here one has to replace the sum-product structures in $f[n]$ for all contributing quantities to their q-extension, see Sections 2 and 3.

Let

$$\mathfrak{A}_G = \{f_1(x), \ldots f_m(x)\}, \qquad x \in]0,1[, \tag{4.2}$$

be an alphabet of functions, which are not higher transcendental. An iterated integral is defined by

$$G\left(\{f_b(\tau), f_{a_1}(\tau), ...f_{a_k}(\tau)\}; x\right) = \int_0^x dy f_b(y) G\left(\{f_{a_1}(\tau), ...f_{a_k}(\tau)\}; y\right) = \sum_{n=1}^{\infty} f[n] x^n. \tag{4.3}$$

The q-extension of G is obtained by

$$G\left(\{f_b(\tau), f_{a_1}(\tau), ...f_{a_k}(\tau)\}; x\right)_q = \sum_{n=1}^{\infty} f[n;q] x^n. \tag{4.4}$$

The hierarchy of iterated integrals is described by the differential equation

$$\frac{d}{dx} G\left(\{f_b(\tau), f_{a_1}(\tau), ...f_{a_k}(\tau)\}; x\right) = f_b(x) G\left(\{f_{a_1}(\tau), ...f_{a_k}(\tau)\}; x\right) \tag{4.5}$$

and for their q-extension by

$$\mathcal{D}_x^q G\left(\{f_b(\tau), f_{a_1}(\tau), ...f_{a_k}(\tau)\}; x\right)_b = \left\{ \frac{d}{dx} G\left(\{f_b(\tau), f_{a_1}(\tau), ...f_{a_k}(\tau)\}; x\right) \right\}_q. \tag{4.6}$$

The definition of the q-free iterated integrals being considered in the following has been given in Ref. [178]. The iterated integrals obey q-differential equations, which can be derived algorithmically. The order of these equations rises with the weight of the corresponding iterated integrals.

Now we turn to the individual classes of iterated integrals: the polylogarithm [158–160], the Nielsen integrals [161,162], harmonic polylogarithms [163], generalized harmonic polylogarithms, also called Kummer-Poincaré integrals [164–172], cyclotomic iterated integrals [173], iterated integrals implied by quadratic forms [174], and iterated integrals containing square-root valued letters [175].

4.1 The q-extended polylogarithm

The polylogarithms [158–160] are iterated integrals over the alphabet

$$\mathfrak{A}_P = \{f_0(x), f_1(x)\} = \left\{ \frac{1}{x}, \frac{1}{1-x} \right\}, \tag{4.7}$$

as in terms of harmonic polylogarithms [163] (see also Section 4.3),

$$\mathrm{Li}_k(x) = \mathrm{H}_{\underbrace{0,\ldots,0}_{k-1},1}(x), \tag{4.8}$$

with

$$\mathrm{Li}_k(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^k}, \quad k \geq 1, \quad x \in [-1,1]. \tag{4.9}$$

The function $f[n]$ for polylogarithms $\mathrm{Li}_k(x)$ is

$$f[n] = \frac{1}{n^k}, \quad k \in \mathbb{Z}, \quad n \in \mathbb{N}\backslash\{0\}. \tag{4.10}$$

The polylogarithms for non-positive index k are given by

$$\mathrm{Li}_0(x) = \frac{x}{1-x}, \tag{4.11}$$

$$\mathrm{Li}_{-k}(x) = \frac{1}{(1-x)^{k+1}} \sum_{l=0}^{k-1} A_{k,l} x^{k-l}, \quad k \geq 1, \tag{4.12}$$

where $A_{k,l}$ are the Eulerian numbers [229]

$$A_{k,l} = (k-l)A_{k-1,l-1} + (k+1)A_{n-1,k}, \quad A_{0,0} = 1, \; A_{0,k} = 0, k \neq 0. \tag{4.13}$$

Polylogarithms for $k > 0$ obey homogeneous differential equations of order $k+1$. The first in the series are

$$\left[-(1-x)\frac{d^2}{dx^2} + \frac{d}{dx}\right] \mathrm{Li}_1(x) = 0, \tag{4.14}$$

$$\left[-(1-x)x\frac{d^3}{dx^3} + (-2+3x)\frac{d^2}{dx^2} + \frac{d}{dx}\right] \mathrm{Li}_2(x) = 0, \tag{4.15}$$

$$\left[-(1-x)x^2\frac{d^4}{dx^4} + (-5+6x)x\frac{d^3}{dx^3} + (-4+7x)\frac{d^2}{dx^2} + \frac{d}{dx}\right] \mathrm{Li}_3(x) = 0. \tag{4.16}$$

The q-extended polylogarithms are defined by

$$\mathrm{Li}_k(x;q) = \sum_{n=1}^{\infty} \frac{x^n}{\{n\}_q^k} = \sum_{n=1}^{\infty} x^n \left[\frac{(1-q)}{(1-q^n)}\right]^k. \tag{4.17}$$

This representation also allows one to define the q-ζ values, the extensions of the Riemann-ζ values,[9]

$$\lim_{x\to 1^-} \mathrm{Li}_k(x;q) = \zeta_k(q) = \sum_{n=1}^{\infty} \frac{1}{\{n\}_q^k} = \sum_{n=1}^{\infty} \left[\frac{(1-q)}{(1-q^n)}\right]^k, \quad k \geq 2, \quad q \in (0,1], \tag{4.18}$$

unlike the case for the μ-extension in Ref. [178].[10] The usual ζ-values are obtained in the limit $q \to 1^-$.

[9] In other approaches additional q-numerator powers are considered. This allows one to expand in q because of the condition Eq. (2.1), cf. Ref. [230]. In our representation for infinite sums the limit $q \to 0$ has to be excluded.

[10] Note, however, that a different version of μ-extension has been used in Refs. [130, 231]. There the values of μ-ζ exist and are used in determining the critical temperature of μ Bose-gas condensation.

By applying the q-derivative to $\mathrm{Li}_k(x;q)$ one obtains

$$x\mathcal{D}_x^q \mathrm{Li}_k(x;q) = \mathrm{Li}_{k-1}(x;q), \tag{4.19}$$

with

$$\mathrm{Li}_1(x;q) = -\ln(1-x)|_q = \sum_{n=1}^{\infty} x^n \frac{(1-q)}{(1-q^n)} \tag{4.20}$$

and for non-positive values of k one can resum the infinite series and obtains

$$\begin{aligned}
\mathrm{Li}_0(x;q) &= \frac{x}{(1-x)} \equiv \mathrm{Li}_0(x), && (4.21)\\
\mathrm{Li}_{-1}(x;q) &= \frac{x}{(1-x)(1-qx)}, && (4.22)\\
\mathrm{Li}_{-2}(x;q) &= \frac{x(1+qx)}{(1-x)(1-qx)(1-q^2x)}, && (4.23)\\
\mathrm{Li}_{-3}(x;q) &= \frac{x(1+2qx+2q^2x+q^3x^2)}{(1-x)(1-qx)(1-q^2x)(1-q^3x)}, && (4.24)
\end{aligned}$$

etc.

For $k > 0$ one obtains the following representation in terms of q-extended generalized hypergeometric functions

$$\mathrm{Li}_k(x;q) = x \cdot {}_{k+1}\phi_k \left(\begin{matrix} q, \ldots, q \\ q^2, \ldots, q^2 \end{matrix}; q, x \right) = \sum_{n=0}^{\infty} \frac{\overbrace{(q;q)_n \cdots (q;q)_n}^{k}}{\underbrace{(q^2;q)_n \cdots (q^2;q)_n}_{k}} x^{n+1}; k \geq 1. \tag{4.25}$$

The recurrence of the expansion coefficients of the q-polylogarithms are

$$(1-q^n)^k f[n;q] - (1-q^{n+1)})^k f[n+1;q] = 0; \quad f[1;q] = 1, \quad k \geq 1. \tag{4.26}$$

Examples of the differential equations for $\mathrm{Li}_k(x;q)$ are[11]

$$\begin{aligned}
((qx-1)\mathcal{D}_x^q + 1)\,\mathrm{Li}_1(x;q) &= \frac{1}{x-1}, \\
\mathrm{Li}_1(0;q) &= 0, && (4.27)\\
\left(qx\left(q^2x-1\right)(\mathcal{D}_x^q)^2 + (q(q+2)x-1)\mathcal{D}_x^q + 1\right)\mathrm{Li}_2(x;q) &= \frac{1}{x-1}, \\
\mathrm{Li}_2(0;q) = 0, \quad \mathcal{D}_x^q \mathrm{Li}_2(0;q) &= 1 && (4.28)\\
\Big[qx\left(q^2x\left(q^3x\left(q^3x-1\right)(\mathcal{D}_x^q)^3 + (q((q(q(q+2)+3)+3)qx-q-2)-3)(\mathcal{D}_x^q)^2\right)\right. & \\
\left. +(q(q(q(q(q+3)+6)+6)+3)x-q(q+3)-3)\mathcal{D}_x^q) + \left((q+1)^3x-1\right)\Big]\mathrm{Li}_3(x;q) &= \frac{1}{x-1}, \\
\mathrm{Li}_3(0;q) = 1,\ \mathcal{D}_x^q \mathrm{Li}_3(0;q) &= 1 + \frac{1}{(q+1)^3},
\end{aligned}$$

[11] Based on the q-recurrences one may find the associated q-differential equations by the command `qREToqDE` and the q-shift relations by `qRETOqSE`, Ref. [217] or by related commands in Ref. [218].

$$(\mathcal{D}_x^q)^2 \mathrm{Li}_3(0;q) = 1 + q + \frac{1}{(q+1)^2} + \frac{q+1}{\left(q^2+q+1\right)^3}. \tag{4.29}$$

The differential equations also apply to Eq. (4.25).

The corresponding q-shift relations for $\mathrm{Li}_k(x;q)$, $k = 1,2,3$, are given by

$$\begin{aligned}
(1-x)(qx-1)F[qx] + (x-1)^2 F[x] + (q-1)x &= 0, && (4.30)\\
(1-x)\left(q^2x-1\right)F[q^2x] + 2(x-1)(qx-1)F[qx] - (x-1)^2F[x] + (q-1)^2x &= 0, && (4.31)\\
q^3(x-1)\left(q^3x-1\right)F\left(q^3x\right) - 3q^2(x-1)\left(q^2x-1\right)F\left(q^2x\right) & \\
+3q(x-1)(qx-1)F(qx) - (x-1)^2F(x) - (q-1)^3 &= 0. && (4.32)
\end{aligned}$$

Quantum dilogarithms were considered in the 1990s in Refs. [232, 233]. The q-logarithm dates back to Euler [234]. Compared to our definition of $\mathrm{Li}_k(x;q)$, deviating representations are used in the literature. Ref. [235] uses a variant of the q-dilogarithm defined by

$$\tilde{\mathrm{Li}}_2(x;q) = \sum_{n=1}^{\infty} \frac{x}{n} \frac{1-q}{1-q^n}, \tag{4.33}$$

and analogously for the polylogarithm in Ref. [236]. Our convention has been used in Ref. [237] for the multiple polylogarithm [238], up to factors of $(1-q)^k$. In Ref. [239] the q-multiple polylogarithm [240] is defined using the symmetric q extension, see Ref. [178], Appendix A, up to factors $(1-q)^k$. Further powers of q are introduced in the numerators of the summands in Ref. [241] for the related q-multiple zeta values, see also Refs. [230, 242–244].

4.2 The q-deformed Nielsen integrals

The Nielsen integrals [161, 162] are the iterative integrals

$$S_{n,p}(x) = \mathrm{H}_{\underbrace{0,\ldots,0}_{n},\underbrace{1,\ldots,1}_{p}}(x), \tag{4.34}$$

over $\mathfrak{A}_P$ written as a harmonic polylogarithm. They can be represented by

$$S_{n,p}(x) = \sum_{k=p}^{\infty} \left[\begin{array}{c} k \\ p \end{array} \right] \frac{x^k}{k^{n+1}} \tag{4.35}$$

by their expansion around $x = 0$. Here the Stirling numbers of the first kind in the notation of Refs. [162, 245, 246] are expressed as modified Faa di Bruno-Ramanujan determinants [177, 247, 248]

$$\left[\begin{array}{c} k \\ p \end{array} \right] = \frac{1}{(p-1)!} \left| \begin{array}{ccccccc}
S_1(k-1) & 1 & 0 & 0 & 0 & ... & 0 \\
S_2(k-1) & S_1(k-1) & 2 & 0 & 0 & ... & 0 \\
S_3(k-1) & S_2(k-1) & S_1(k-1) & 3 & 0 & ... & 0 \\
\vdots & & & & & & \vdots \\
S_{p-1}(k-1) & ... & & & & ... & S_1(k-1)
\end{array} \right|, \quad p > 1; \tag{4.36}$$

$$\left[\begin{array}{c} k \\ 1 \end{array} \right] = (k-1)!, \quad \left[\begin{array}{c} k \\ 0 \end{array} \right] = \delta_{0k}, \tag{4.37}$$

with

$$\left[\begin{array}{c} k \\ p \end{array} \right] = s(k,p)\frac{(-1)^k}{(k-1)!}. \tag{4.38}$$

Furthermore, one has

$$S_{0,p} = \frac{1}{p!}\ln^p(1-x). \tag{4.39}$$

Nielsen integrals of weight $\mathsf{w} = n+p$ obey differential equations of order $n+p+1$. Examples are

$$\left[x(x-1)^2\frac{d^4}{dx^4} + 3(2x-1)(x-1)\frac{d^3}{dx^3} + (7x-6)\frac{d^2}{dx^2} + \frac{d}{dx}\right] S_{1,2}(x) = 0, \tag{4.40}$$

$$\left[x(x-1)^3\frac{d^5}{dx^5} + 2(5x-2)(x-1)^2\frac{d^4}{dx^4} + (25x-18)(x-1)\frac{d^3}{dx^3} + (15x-14)\frac{d^2}{dx^2} + \frac{d}{dx}\right] \times S_{1,3}(x) = 0, \tag{4.41}$$

$$\left[(1-x)^2x^2\frac{d^5}{dx^5} + (x-1)(10x-7)x\frac{d^4}{dx^4} + \left(25x^2-33x+9\right)\frac{d^3}{dx^3} + 3(5x-4)\frac{d^2}{dx^2} + \frac{d}{dx}\right] \times S_{2,2}(x) = 0. \tag{4.42}$$

The q-extension $S_{n,p}(x;q)$ is obtained by

$$S_{n,p}(x;q) \;=\; \sum_{k=p}^{\infty} \left[\begin{array}{c} k \\ p \end{array} \right]_q \left[\frac{(1-q)}{(1-q^k)}\right]^{n+1} x^k, \tag{4.43}$$

with

$$\left[\begin{array}{c} k \\ p \end{array} \right]_q = \left[\begin{array}{c} k \\ p \end{array} \right] \{S_l(k-1) \to S_l(k-1;q)\}, \quad l \geq 1, l \in \mathbb{N}. \tag{4.44}$$

The hierarchy equations for the q-extended Nielsen integrals are

$$x\mathcal{D}_x^{(q)} S_{n,p}(x;q) \;=\; S_{n-1,p}(x;q). \tag{4.45}$$

The expansion coefficients $f[n;q]$ for $S_{1,2}(x;q), S_{1,3}(x;q)$ and $S_{2,2}(x;q)$ obey the recurrences

$$-\left(1-q^n\right)^3 f[n;q] - \left(1-q^{1+n}\right)^2\left(-2+q^n+q^{1+n}\right) f[n+1,q] - \left(1-q^{1+n}\right)\left(1-q^{2+n}\right)^2 \times f[n+2;q] = 0, \tag{4.46}$$

$$\left(q^n-1\right)^4 f[n;q] - \left(q^{n+1}-1\right)^2\left(-3(q+1)q^n + \left(q^2+q+1\right)q^{2n} + 3\right) f[n+1;q] + \left(q^{n+1}-1\right)\left(q^{n+2}-1\right)^2\left(\left(q^2+q+1\right)q^n - 3\right) f[n+2;q] + \left(1-q^{n+1}\right)\left(q^{n+2}-1\right) \times \left(q^{n+3}-1\right)^2 f[n+3;q] = 0, \tag{4.47}$$

$$\left(1-q^n\right)^4 f[n;q] + \left(1-q^{1+n}\right)\Big[\left(1-q^{1+n}\right)^2\left(-2+q^n+q^{1+n}\right) f[n+1;q] + \left(1-q^{2+n}\right)^3 f[n+2;q]\Big] = 0. \tag{4.48}$$

The initial conditions are obtained by the first expansion coefficients of (4.43). The q-differential equations for $S_{1,2}(x;q), S_{1,3}(x;q)$ and $S_{2,2}(x;q)$ are

$$\Big[q^3x\left(q^2x-1\right)(\mathcal{D}_x^{(q)})^4+(qx-1)\left(q^4x+2q^3x+q^2(3x-1)-q-1\right)(\mathcal{D}_x^{(q)})^3$$
$$+\left(q^3x+q^2(3x-1)+3q(x-1)-2\right)(\mathcal{D}_x^{(q)})^2+\mathcal{D}_x^{(q)}\Big]F[x]=0$$
$$F[0]=\mathcal{D}_x^{(q)}F[0]=0,(\mathcal{D}_x^{(q)})^2F[0]=\frac{1}{1+q},(\mathcal{D}_x^{(q)})^3F[0]=\frac{2+q}{1+q+q^2}. \tag{4.49}$$
$$\Big[q^4x\left(q^3x-1\right)(q^2x-1)(\mathcal{D}_x^{(q)})^5+\left(q^2x-1\right)\left(q^6x+2q^5x+3q^4x+q^3(4x-1)-q^2\right.$$
$$\left.-q-1\right)(\mathcal{D}_x^{(q)})^4+(qx-1)\left(q^6x+3q^5x+q^4(7x-1)+q^3(8x-3)+6q^2(x-1)-5q-3\right)$$
$$\times(\mathcal{D}_x^{(q)})^3+\left(q^4x+q^3(4x-1)+q^2(6x-4)+q(4x-6)-3\right)(\mathcal{D}_x^{(q)})^2+\mathcal{D}_x^{(q)})\Big]F[x]=0,$$
$$F[0]\;=\;\mathcal{D}_x^{(q)}F[0]\;=\;(\mathcal{D}_x^{(q)})^2F[0]\;=\;0,(\mathcal{D}_x^{(q)})^3F[0]\;=\;\frac{2}{1+q+q^2},$$
$$(\mathcal{D}_x^{(q)})^4F[0]\;=\;\frac{2(3+2q+q^2)}{(1+q)(1+q^2)}, \tag{4.50}$$
$$\Big[q^7x^2(qx-1)\left(q^2x-1\right)(\mathcal{D}_x^{(q)})^5+q^3x(qx-1)\left(q^5x+2q^4x+q^3(3x-1)+q^2(4x-2)\right.$$
$$\left.-2q-2\right)(\mathcal{D}_x^{(q)})^4+\left(q^7x^2+q^6x(3x-1)+q^5x(7x-4)+q^4\left(8x^2-9x+1\right)\right.$$
$$\left.+q^3\left(6x^2-11x+2\right)+q^2(3-7x)-q(x-2)+1\right)(\mathcal{D}_x^{(q)})^3+(q+2)\left(q^3x+q^2(2x-1)\right.$$
$$\left.+2q(x-1)-1\right)(\mathcal{D}_x^{(q)})^2+\mathcal{D}_x^{(q)}\Big]F(x)=0,$$
$$F(0)=\mathcal{D}_x^{(q)}F(0)=0,(\mathcal{D}_x^{(q)})^2F(0)=\frac{1}{(1+q)^2},(\mathcal{D}_x^{(q)})^3F(0)=\frac{2+q}{(1+q+q^2)^2},$$
$$(\mathcal{D}_x^{(q)})^4F(0)=\frac{3+4q+3q^2+q^3}{(1+q)^2(1+q^2)^2}. \tag{4.51}$$

The associated q-shift relations for $S_{1,2}(x;q), S_{1,3}(x;q)$ and $S_{2,2}(x;q)$ are

$$q^3(x-1)^2F[x]-q\left(q^2\left(4x^2-5x+2\right)-3qx+q+1\right)F[qx]+\left(q^3\left(6x^2-4x+1\right)\right.$$
$$\left.+q^2(2-7x)-q(x-2)+1\right)F[q^2x]-(qx-1)\left(q^2(4x-1)-q-2\right)F[q^3x]$$
$$+(qx-1)\left(q^2x-1\right)F[q^4x]=0, \tag{4.52}$$
$$-q^6(x-1)^3F(x)+q^3\left(q^3\left(5x^3-9x^2+7x-2\right)+q^2\left(-6x^2+4x-1\right)+q(4x-1)-1\right)$$
$$\times F[qx]-q\left(q^5\left(10x^3-10x^2+5x-1\right)+q^4\left(-16x^2+9x-2\right)-2q^3\left(2x^2-5x+1\right)\right.$$
$$\left.+q^2(5x-3)+q(x-1)-1\right)F[q^2x]+(qx-1)\left(q^5\left(10x^2-5x+1\right)+q^4(1-5x)+q^3(3-9x)\right.$$
$$\left.-q^2(x-2)+2q+1\right)F[q^3x]-(qx-1)\left(q^2x-1\right)\left(q^3(5x-1)-q^2-q-2\right)F[q^4x]$$
$$+(qx-1)\left(q^2x-1\right)\left(q^3x-1\right)F[q^5x]=0, \tag{4.53}$$
$$-q^3(x-1)^2F[x]+q\left(q^2\left(5x^2-7x+3\right)-3qx+q+1\right)F[qx]+\left(q^3\left(-10x^2+9x-3\right)\right.$$
$$\left.+q^2(10x-3)+q(x-3)-1\right)F[q^2x]+\left(q^3\left(10x^2-5x+1\right)+q^2(3-12x)-3q(x-1)+3\right)$$
$$\times F[q^3x]-(qx-1)\left(q^2(5x-1)-q-3\right)F[q^4x]+(qx-1)\left(q^2x-1\right)F[q^5x]=0. \tag{4.54}$$

4.3 The q-deformed harmonic polylogarithms

The harmonic polylogarithms [163] are iterated integrals over the alphabet

$$\mathfrak{A}_{\rm H} = \{f_0(x), f_1(x), f_{-1}(x)\} \equiv \left\{\frac{1}{x}, \frac{1}{1-x}, \frac{1}{1+x}\right\}, \tag{4.55}$$

by

$$\mathrm{H}_{b,\vec{a}}(x) = \int_0^x dy f_b(y)\mathrm{H}_{\vec{a}}(y), \quad \mathrm{H}_\emptyset(x) = 1. \tag{4.56}$$

The most simple harmonic polylogarithms are $\mathrm{H}_{-1}(x), \mathrm{H}_1(x), \mathrm{H}_0(x)$. The first two have the following $f[n]$-function

$$f[n]^{(-1)} = \frac{(-1)^n}{n}, \tag{4.57}$$

$$f[n]^{(1)} = \frac{1}{n}, \tag{4.58}$$

from which

$$\mathrm{H}_{-1}(x;q) = \sum_{n=1}^{\infty} \frac{1-q}{1-q^k}(-x)^k = x \cdot {}_2\phi_1\left(\begin{matrix}q, q\\ q^2\end{matrix}; q, -x\right), \tag{4.59}$$

$$\mathrm{H}_1(x;q) = \sum_{n=1}^{\infty} \frac{1-q}{1-q^k}x^k = x \cdot {}_2\phi_1\left(\begin{matrix}q, q\\ q^2\end{matrix}; q, x\right) \tag{4.60}$$

are obtained. This yields the representation

$$\mathrm{H}_0(x;q) = -\sum_{n=1}^{\infty} \frac{1-q}{1-q^k}(1-x)^k. \tag{4.61}$$

Due to the complexity of the iterative integrals by growing alphabets and permutation of letters in this and the following cases, we will refer to characteristic examples henceforth. Let us consider the harmonic polylogarithm $\mathrm{H}_{-1,0,1}(x)$. Its function $f[n]$ is given by

$$f[n] = \left[\frac{1}{n^3} - \frac{(-1)^n}{n}S_{-2}(n)\right]. \tag{4.62}$$

The differential equation for $\mathrm{H}_{-1,0,1}(x)$ reads

$$\left[-(1-x)x(1+x)\frac{d^4}{dx^4} + 2(-1-x+3x^2)\frac{d^3}{dx^3} + (-3+7x)\frac{d^2}{dx^2} + \frac{d}{dx}\right]\mathrm{H}_{-1,0,1}(x) = 0. \tag{4.63}$$

The q-extension of Eq. (4.62) is given by

$$f[n;q] = (1-q)^3\left[\frac{1}{(1-q^n)^3} - \frac{(-1)^n}{(1-q^n)}\sum_{k=1}^{n}\frac{(-1)^k}{(1-q^k)^2}\right]. \tag{4.64}$$

It obeys the recurrence

$$-\left(q^n-1\right)^3 f[n,q] + (q-1)\left(q^{n+1}-1\right)\left(q^{n+1}+q^n-2\right)q^n f[n+1;q]$$

$$+\left(q^{n+1}-1\right)^2\left(q^{n+2}-1\right)f[n+2;q]=0. \tag{4.65}$$

The q-extension of the derivative of $\mathrm{H}_{-1,0,1}(x)$, $\mathrm{H}_{0,1}(x)/(1+x)$, is

$$f^{(1)}[n;q]=(-1)^n\sum_{k=1}^{n}(-1)^k\frac{(1-q)^2}{(1-q^k)^2}. \tag{4.66}$$

Here the hierarchy-equation is

$$\mathcal{D}_x^{(q)}\mathrm{H}_{-1,0,1}(x;q)=\left[\frac{1}{1+x}\,\mathrm{H}_{0,1}(x)\right]\Big|_q. \tag{4.67}$$

The q-extended harmonic polylogarithm $\mathrm{H}_{-1,0,1}(x)$ obeys

$$\begin{aligned}&\Big[\mathcal{D}_x^{(q)}+q\left[q^2x+q(3x-1)+3x-2\right](\mathcal{D}_x^{(q)})^2+\left[q^5x^2+q^4x(2x-1)+q^3x(3x-2)\right.\\&\left.-q^2x+q(2x-1)-1\right](\mathcal{D}_x^{(q)})^3+q^2x(qx-1)\left(q^3x+1\right)(\mathcal{D}_x^{(q)})^4\Big]F[x]=0,\end{aligned} \tag{4.68}$$

with

$$F[0]\;=\;\mathcal{D}_x^{(q)}\;F[0]\;=0,\quad(\mathcal{D}_x^{(q)})^2\;F[0]=1,\quad(\mathcal{D}_x^{(q)})^3\;F[0]=-\frac{q(q+2)}{q+1}. \tag{4.69}$$

The q-shift relation is given by

$$\begin{aligned}&q^4(x-1)(x+1)F[x]+q^2\left(q^2\left(-4x^2+2x+1\right)-2q(x-1)+1\right)F[qx]\\&+q\left(3q^3x(2x-1)-2q^2+q(3x-2)-2\right)F\left[q^2x\right]+\left(q^4\left(x-4x^2\right)+3q^3x+q^2(1-3x)\right.\\&\left.-q(x-2)+1\right)F\left[q^3x\right]+(qx-1)\left(q^3x+1\right)F\left[q^4x\right]=0.\end{aligned} \tag{4.70}$$

Similar relations hold for all q-extended harmonic polylogarithms.

The q-multiple zeta values can be obtained from the q-extended harmonic polylogarithms for $x=1$ like for the multiple zeta values [249] from the harmonic polylogarithms,

$$\zeta_{-1,0,1}(q)=\mathrm{H}_{-1,0,1}(1;q)=\sum_{k=1}^{\infty}f[k;q]. \tag{4.71}$$

In the limit $q\to 1^-$, $\zeta_{-1,0,1}(q)$ approaches

$$\mathrm{H}_{-1,0,1}(1)=\ln(2)\zeta_2-\frac{5}{8}\zeta_3. \tag{4.72}$$

4.4 The *q*-deformed generalized harmonic polylogarithms

We consider the q-extension of the generalized harmonic polylogarithms, cf. Refs. [171,172]. The function $\mathrm{H}[-1/2,2,-1,x]$ is a typical example. We calculate it algorithmically. The associated function $f[n]$ reads

$$f[n]=\frac{(-1)^n}{n^3}-\frac{2^{-n}}{n^2}S_1(-2,n)-\frac{(-2)^n}{n}S_2\left(\frac{1}{2},n\right)+\frac{(-2)^n}{n}S_{1,1}\left(-\frac{1}{4},-2,n\right), \tag{4.73}$$

cf. Ref. [178]. The q-extension is

$$
\begin{aligned}
f[n;q] = & \\
& (-1)^n \left(\frac{1-q}{1-q^n}\right)^3 - 2^{-n} \left(\frac{1-q}{1-q^n}\right)^2 \sum_{k=1}^{n} (-1)^k \left(\frac{1-q}{1-q^k}\right) \\
& -(-2)^n \left(\frac{1-q}{1-q^n}\right) \sum_{k=1}^{n} \left(\frac{1}{2}\right)^k \left(\frac{1-q}{1-q^k}\right)^2 + (-2)^n \left(\frac{1-q}{1-q^n}\right) \\
& \times \sum_{k=1}^{n} \left(-\frac{1}{4}\right)^k \left(\frac{1-q}{1-q^k}\right) \sum_{l=1}^{k} (-2)^l \left(\frac{1-q}{1-q^l}\right) \\
= \; & (-2)^n \left(\frac{1-q}{1-q^n}\right) \sum_{k=1}^{n-1} \left\{ \left(-\frac{1}{4}\right)^k \left(\frac{1-q}{1-q^k}\right) \sum_{l=1}^{k} (-2)^l \left(\frac{1-q}{1-q^l}\right) - \left(\frac{1}{2}\right)^k \left(\frac{1-q}{1-q^k}\right)^2 \right\}.
\end{aligned}
\tag{4.74}
$$

The function $F[x;q]$, cf. Eq. (1.3), starts $\propto x^3$.

Here and in the following it is useful to determine the recurrences for the individual terms first. Afterwards these recurrences are combined into a single recurrence. Furthermore, the use of formal parameters for the power-terms is usually faster then considering the special ones. Therefore one sets, e.g., $(-2)^k \equiv a^k$, etc. This also avoids complex algebra in some of the examples discussed below.

Let us consider the example

$$
T_1[n] = \sum_{k=1}^{n} c^k \left(\frac{1-q}{1-q^k}\right)^2, \quad c \in \mathbb{C}\backslash\{0\}. \tag{4.75}
$$

It obeys the recurrence

$$
\begin{aligned}
& c\left(q^{n+1}-1\right)^2 T_1[n-1] + \left(2cq^{n+1} - cq^{2(n+1)} - c + 2q^{n+2} - q^{2(n+1)+2} - 1\right) T_1[n] \\
& + \left(q^{n+2}-1\right)^2 T_1[n+1] = 0, \quad n \geq 1,
\end{aligned}
\tag{4.76}
$$

with

$$
T_1[0] = c, \quad T_1[1] = c + \frac{c^2(1-q)^2}{\left(1-q^2\right)^2}. \tag{4.77}
$$

The recurrence for $f[n;q]$ is obtained by

$$
\begin{aligned}
& 2\left(q^n-1\right)^3 f[n;q] + \left(q^{n+1}-1\right)\left(q^n\left((2(q-2)q+1)q^n+2\right)-1\right) f[n+1;q] \\
& + \left(q^{n+1}-1\right)\left(1-q^{n+2}\right)\left((q(4q-1)+2)q^n-5\right) f[n+2;q] \\
& +2\left(q^{n+1}-1\right)\left(1-q^{n+2}\right)\left(q^{n+3}-1\right) f[n+3;q] = 0,
\end{aligned}
\tag{4.78}
$$

with

$$
f[0;q] = f[1;q] = f[2;q] = 0, f[3;q] = \frac{1}{1+2q+2q^2+q^3}. \tag{4.79}
$$

The related q-shift relation reads

$$
q^6(x-2)(x+1)(2x+1)F(x) - q^3(q(q(q(x(x+1)(8x-9)-2)-x(3x+4)-2)-7x-2)
$$

$$-2)F(qx)+q\left(12q^5x^3+(q(2q-7)-1)q^3x^2-2\left(q^2+q+1\right)(2q(q+1)+1)qx\right.$$
$$\left.-2\left(q\left(q^2+q+2\right)+1\right)q-2\right)F\left(q^2x\right)+\left(-8q^6x^3+(q(5-2(q-1)q)-1)q^3x^2\right.$$
$$\left.+\left((q(4q+3)+10)q^2+q+2\right)qx+2\left(q^2+q+1\right)q+2\right)F\left(q^3x\right)+(qx+1)\left(q^2x-2\right)$$
$$\left(2q^3x+1\right)F\left(q^4x\right)=0, \tag{4.80}$$

with

$$\langle 1\rangle[F(x)]=0,\quad \langle x\rangle[F(x)]=0,\qquad \left\langle x^2\right\rangle[F(x)]=0,\qquad \left\langle x^3\right\rangle[F(x)]=\frac{1}{(q+1)\left(q^2+q+1\right)}. \tag{4.81}$$

The q-differential equation reads

$$\left[(qx+1)\left(q^2x-2\right)\left(2q^3x+1\right)(\mathcal{D}_x^q)^4+(q(q(x(2q((q(q+2)+3)x+q)-3)-4)-2x-3)\right.$$
$$\left.-5)(\mathcal{D}_x^q)^3+(2q((q(q+3)+3)x+q)-1)(\mathcal{D}_x^q)^2+2\mathcal{D}_x^q\right]F[x;q]=0, \tag{4.82}$$

where

$$F[0]=F^{(1)}[0]=F^{(2)}[0]=0. \tag{4.83}$$

The expansion coefficient of the derivative of $\mathrm{H}[-1/2,2,-1,x]$, $2\mathrm{H}[2,-1,x]/(1+2x)$, is

$$f[n]=(-2)^{1+n}\left[S_{1,1}\left(-\frac{1}{4},-2,n\right)-S_2\left(\frac{1}{2},n\right)\right], \tag{4.84}$$

resulting into

$$f^{(1)}[n;q]=(-2)^{1+n}\left[\sum_{k=1}^{n}\left(-\frac{1}{4}\right)^k\frac{(1-q)}{(1-q^k)}\sum_{l=1}^{k}(-2)^l\frac{(1-q)}{(1-q^l)}-\sum_{k=1}^{n}\left(\frac{1}{2}\right)^k\left(\frac{1-q}{1-q^k}\right)^2\right]. \tag{4.85}$$

The hierarchy equation follows from Eqs. (2.3, 4.74) and (4.85) by

$$\mathcal{D}_x^q\sum_{n=0}^{\infty}f[n;q]x^n=\sum_{n=1}^{\infty}f[n;q]\frac{1-q^n}{1-q}x^{n-1}. \tag{4.86}$$

4.5 The q-deformed cyclotomic harmonic polylogarithms

We consider the following cyclotomic harmonic polylogarithm, cf. Ref. [173],

$$\mathrm{G}\left[\left\{\frac{1}{1-\tau+\tau^2},\frac{1}{1+\tau}\right\},x\right] \tag{4.87}$$

as an instructive example and construct its q-extension. The associated function $f[n]$ is obtained by

$$f[n] \;=\; -\frac{(-1)^{2/3}\left(-(-1)^{2/3}\right)^n}{\left(1+\sqrt[3]{-1}\right)n}S_1\left(-\sqrt[3]{-1},n\right)+\frac{(-1)^{2/3+n/3}}{\left(1+\sqrt[3]{-1}\right)n}S_1\left((-1)^{2/3},n\right), \tag{4.88}$$

cf. Ref. [178], with

$$f[n;q] \;=\; \frac{a^2}{\left(1+a\right)\{n\}_q}\left[-(-a^2)^nS_1\left(-a,n;q\right)+a^nS_1\left(a^2,n;q\right)\right],\quad a\equiv(-1)^{1/3}. \tag{4.89}$$

The recurrence reads

$$-\left(q^n-1\right)\left(q^{n+1}-1\right)f[n;q]-\left(\left(q-1\right)\left(q^{n+1}-1\right)q^{n+1}\right)f[n+1;q]$$
$$+(q-1)\left(q^{n+2}-1\right)q^{n+1}f[n+2;q]-\left(q^{n+2}-1\right)\left(q^{n+3}-1\right)f[n+3;q]=0, \quad (4.90)$$

with

$$f[0;q]=f[1;q]=0. \quad (4.91)$$

The q-shift relation is

$$(1-q)^2qx^2-q\left(x^3+1\right)F[x]+(x+1)\left(q(q+1)x^2-2qx+q+1\right)F[qx]$$
$$-(x+1)(qx(qx-1)+1)F\left[q^2x\right]=0, \quad (4.92)$$

with

$$\langle 1\rangle[F(x)]=\langle x\rangle[F(x)]=0. \quad (4.93)$$

The q-differential equation is

$$\left[(qx(qx-1)+1)(\mathcal{D}_x^q)^2-(x+1)(qx+x-1)\mathcal{D}_x^q\right]F[x;q]=\frac{1}{1+x}, \quad (4.94)$$

with

$$F[0;q]=\mathcal{D}_x^q[F][0;q]=0. \quad (4.95)$$

By applying the q-differential operator one can check the hierarchy also in the present case. One has

$$f^{(1)}[n,q]=-\frac{1}{1+a}\left[a\left(-a^2\right)^nS_1(-a,n)+a^nS_1\left(a^2,n\right)\right]. \quad (4.96)$$

From this it follows

$$\mathcal{D}_x^q\sum_{n=0}^{\infty}f[n;q]x^n=\sum_{n=1}^{\infty}f[n;q]\{n\}_qx^{n-1}, \quad (4.97)$$

cf. Eqs. (4.89) and (4.96).

4.6 The q-deformed harmonic polylogarithms inspired by quadratic forms

An example of this class of iterated integrals is, cf. Ref. [174],

$$T_3=\int_0^x dy_1\frac{1}{y_1^2+y_1-2}\int_0^{y_1}dy_2\frac{1}{y_2+1}\int_0^{y_2}dy_3\frac{1}{y_3-1}$$
$$=\sum_{n=1}^{\infty}\frac{1}{3n}\left[\frac{1}{2}S_2(n)-\frac{1}{2}S_{-1}^2(n)-\left(-\frac{1}{2}\right)^nS_2(-2,n)+\left(-\frac{1}{2}\right)^nS_{1,1}(2,-1,n)\right]x^n. \quad (4.98)$$

The q-extension of the central function $f[n]$ of T_3 reads

$$f[n;q] = \frac{1}{3}\frac{1-q}{1-q^n}\left\{\frac{1}{2}\sum_{k=1}^{n}\left(\frac{1-q}{1-q^k}\right)^2-\frac{1}{2}\left[\sum_{k=1}^{n}(-1)^k\frac{1-q}{1-q^k}\right]^2-\left(-\frac{1}{2}\right)^n\sum_{k=1}^{n}(-2)^k\frac{1-q}{1-q^k}\right.$$

$$+\left(-\frac{1}{2}\right)^n \sum_{k=1}^{n} 2^k \frac{1-q}{1-q^k} \sum_{l=1}^{k} (-1)^l \frac{1-q}{1-q^l}\Bigg\} \tag{4.99}$$

with

$$\{T_3\}_q = \sum_{n=0}^{\infty} f[n;q] x^n. \tag{4.100}$$

The recursion for $f[n,q]$ is of 5th order and has the following structure

$$\begin{aligned}
&q^2(q^n-1)((q^{1+n}-1)^2)(q^{2+n}-1)[p_1(q)+q^n p_2(q)+q^{2n}p_3(q)]f[n;q]\\
&+(q-1)(q^{1+n}-1)(q^{2+n}-1)[p_4(q)+q^n p_5(q)+q^{2n}p_6(q)+q^{3n}p_7(q)+q^{4n}p_8(q)]f[n+1;q]\\
&+(q^{2+n}-1)[p_9(n)+q^n p_{10}(q)+q^{2n}p_{11}(q)+q^{3n}p_{12}(q)+q^{4n}p_{13}(q)+q^{5n}p_{14}(q)]f[n+2;q]\\
&+(q^{3+n}-1)[p_{15}(q)+q^n p_{16}(q)+q^{2n}p_{17}(q)+q^{3n}p_{18}(q)+q^{4n}p_{19}(q)+q^{5n}p_{20}(q)]f[n+3;q]\\
&+(q^{4+n}-1)^2[p_{21}(q)+q^n p_{22}(q)+q^{2n}p_{23}(q)+q^{3n}p_{24}(q)+q^{4n}p_{25}(q)]f[n+4;q]\\
&+2(q^{4+n}-1)(q^{5+n}-1)^3[p_{26}(q)+q^n p_{27}(q)+q^{2n}p_{28}(q)]f[n+5;q]=0,
\end{aligned} \tag{4.101}$$

with large polynomials $p_i(q)$.[12] Analogously to previous cases, one can derive also the q-differential equation and q-shift relation, which also form very large expressions. The hierarchy relation is

$$\mathcal{D}_x^q\{T_3\}_q = \sum_{n=1}^{\infty} f[n;q] \frac{1-q^n}{1-q} x^{n-1}, \tag{4.102}$$

which is equal to the q-extension of the moments of $dT_3/dx = -\mathrm{H}_{-1,1}(x)/(x^2+x-2)$. The analysis of the recurrence Eq. (4.101) by using `Sigma` shows, that the minimal recurrence is actually of order $\mathtt{o} = 4$. The larger recurrence was obtained by joining recurrences for individual summands.

4.7 The q-deformed iterated integrals containing square-root valued letters

Square-root valued iterated integrals have been considered in Refs. [175, 250]. Their Mellin transforms lead to nested sums with central binomials at different places in the numerator or denominator. They arise in higher order perturbative calculations. In particular we refer to the letters (3.25–3.63) of the alphabet given in Ref. [175]. This class of functions is the most involved one found in quantum field theoretical calculations, which still obey first order factorizing differential and difference equations.

As a typical example we consider the q-extension of the function

$$T_4(x) = \sum_{n=1}^{\infty} \frac{4^n}{n^2\binom{2n}{n}} S_1(n) x^n, \tag{4.103}$$

with

$$T_4(x;q) = \sum_{n=1}^{\infty} 4^n \left(\frac{1-q}{1-q^n}\right)^2 \frac{\prod_{k=1}^{n}(1-q^k)^2}{\prod_{k=1}^{2n}(1-q^k)} \sum_{k=1}^{n} \frac{(1-q)}{(1-q^k)}\ x^n = \sum_{n=1}^{\infty} f[n;q] x^n. \tag{4.104}$$

[12] The recurrence is given in computer-readable form as ancillary file to this paper.

We obtain the following recurrence for the function $f[n;q]$

$$16\left(q^n-1\right)^2\left(q^{n+1}-1\right)^2 f[n;q]-4\left(q^{n+1}+1\right)\left(q^{2n+1}-1\right)\left((q+1)q^{n+1}-2\right)\left(q^{n+1}-1\right)^2$$
$$\times f[n+1;q]+\left(q^{n+1}+1\right)\left(q^{n+2}-1\right)^2\left(q^{n+2}+1\right)\left(q^{2n+1}-1\right)\left(q^{2n+3}-1\right)f[n+2;q]=0, \tag{4.105}$$

with

$$f[0;q]=0,\quad f[1;q]=\frac{4}{1+q}. \tag{4.106}$$

In this sense the case of square-root iterated integrals is not different from the other iterated integrals obeying first order factorizing differential equations.

The q-shift relation is given by

$$q^5(1-4x)^2F[x]+Q_1F[qx]+Q_2F[q^2x]+Q_3F[q^3x]+Q_4F[q^4x]+Q_5F[q^5x]$$
$$+Q_6F[q^6x]+(q-1)F[q^7x]+F[q^8x]+8(q-1)^4q^4x=0, \tag{4.107}$$

with the polynomials

$$\begin{aligned}
Q_1 &= -q^4(q(8x-1)(4(q+1)x-1)-1),\\
Q_2 &= q^2\left(q^2(q(4x(4(q(q+4)+1)x-q+1)-1)+8x-2)-1\right),\\
Q_3 &= -q\left(q\left(q(q+1)\left(q\left(4x\left(8q^2x+q+3\right)-1\right)+1\right)-1\right)+1\right),\\
Q_4 &= q\left(q^2\left(4qx\left(q\left(4q^2x+q+2\right)-1\right)+2q+1\right)+q+2\right),\\
Q_5 &= \left(q^2(q(4(q+3)qx-q+1)-1)+1\right),\\
Q_6 &= -\left(4(q+1)q^4x+q^3+2q+1\right).
\end{aligned} \tag{4.108}$$

The initial values for Eq. (4.107) are $\langle x^k\rangle[F[x]]=f[k;q], k\in[0,6]$ given by the first expansion coefficients of $T_4(x;q)$, Eq. (4.104).

The q-differential equation is obtained by

$$\Big\{8+Q_7\mathcal{D}_x^q+Q_8(\mathcal{D}_x^q)^2+Q_9(\mathcal{D}_x^q)^3+Q_{10}(\mathcal{D}_x^q)^4+Q_{11}(\mathcal{D}_x^q)^5+Q_{12}(\mathcal{D}_x^q)^6+Q_{13}(\mathcal{D}_x^q)^7$$
$$+(q-1)^4q^{24}x^7(\mathcal{D}_x^q)^8\Big\}F[x;q]=0, \tag{4.109}$$

with the polynomials

$$\begin{aligned}
Q_7 &= 2(q+1)\left(2q^2x(4x-1)+4qx(2x-1)-1\right),\\
Q_8 &= -(q+1)x\left(4q^7x+q^6(12x-1)-2q^5\left(8x^2-12x+1\right)+q^4\left(-32x^2+28x-3\right)\right.\\
&\quad \left.+q^3\left(-48x^2+28x-3\right)-2q^2\left(8x^2-6x+1\right)-q-2\right),\\
Q_9 &= qx^2(q^{12}+q^{11}(2-4x)+q^{10}(5-12x)+q^9(7-24x)+q^8(11-40x)\\
&\quad +4q^7\left(4x^2-12x+3\right)+q^6\left(32x^2-48x+13\right)+q^5\left(48x^2-28x+9\right)\\
&\quad +q^4\left(32x^2-8x+6\right)+q^3(12x+1)+8q^2x-q-2),\\
Q_{10} &= q^3x^3(q^{15}+q^{14}+2q^{13}-4q^{12}(x-1)+q^{11}(5-8x)+q^{10}(5-12x)\\
&\quad +q^9(7-16x)+q^8(4-16x)+q^7(2-4x)+16q^6x^2+q^5(8x-3)+2q^4(8x-3)\\
&\quad +q^3(4x-2)-3q^2-2q+1),
\end{aligned}$$

$$
\begin{aligned}
Q_{11} &= (q-1)q^7x^4(q^{14}+q^{13}+2q^{12}+3q^{11}+5q^{10}+q^9(5-4x)+q^8(7-8x)\\
&\quad +q^7(5-8x)+q^6(6-8x)+q^5(3-8x)+q^4(1-4x)+q^3(8x-2)-3q-2),\\
Q_{12} &= (q-1)^2q^{11}x^5(q^{12}+q^{11}+2q^{10}+2q^9+3q^8+4q^7\\
&\quad +4q^6+q^5(3-4x)+q^4(3-4x)+q^3+2q^2-q-1),\\
Q_{13} &= (q-1)^3\left(q^6+q^5+q^4+q^3+q^2+q+2\right)q^{18}x^6,
\end{aligned}
\tag{4.110}
$$

where $(\mathcal{D}_x^q)^k F[0;q] = \{n!\}_q f[k;q], \quad k \in [1,7]$.

Given the complexity of the expression (4.104) compared to other cases discussed before, the recurrence is small. However, much larger q-shift and q-differential equations are obtained. In the same way as for (4.104) one may solve more involved cases, leading to larger determining equations.

With this we have found for all presently known first order factorizing solutions of special functions emerging in higher order calculations of single scale Feynman diagrams the respective q-extensions, either in general form or by algorithmic steps to be applied to the respective cases. They are uniquely defined by their q-recursion relations, their q-differential equations, and q-shift relations.

5 Shuffle and quasi-shuffle algebras

Also in the case of q-deformed iterated integrals and nested sums the products of the respective quantities can be described by shuffle and quasi-shuffle relation, cf. Refs. [171,177,251,252], since these are purely index-based and induced by the respective alphabets.

The products of two iterated integrals $G_{a_1,...,a_l}(x)$ and $G_{b_1,...,b_m}(x)$ is the sum of all iterated integrals of weight $l+m$ over all shuffles

$$
\{\{c_1,...,c_{l+m}\}\} = \{a_1,...,a_l\} \sqcup\!\sqcup \{b_1,...,b_m\}, \tag{5.1}
$$

where the shuffle product is denoted by $\sqcup\!\sqcup$. The indices a_i, b_j refer to the alphabet $\mathfrak{A}_F$ of functions to be iterated, where the order of letters of the set $\{a_1,...,a_l\}$ and $\{b_1,...,b_m\}$ is preserved, while all other combinations are allowed,

$$
G_{a_1,...,a_l}(x) \cdot G_{b_1,...,b_m}(x) = \sum_{C \in \{\{c_1,...,c_{l+m}\}\}} G_C(x). \tag{5.2}
$$

The nested sums obey quasi-shuffle products, since there are additional trace terms, cf. Refs. [171, 252], which apply also to their q-extension. We illustrate the principal structure for the q-extended generalized harmonic sums. For the product of q-extended generalized harmonic sums, $S_{a_1,...,a_l}(c_1,...,c_l;N;q)$ and $S_{b_1,...,b_m}(d_1,...,d_m;N;q)$, one obtains

$$
\begin{aligned}
&S_{a_1,...,a_l}(c_1,...,c_l;N;q) \cdot S_{b_1,...,b_m}(d_1,...,d_m;N;q) = \\
&\qquad \sum_{n=1}^{N} \frac{c_1^n}{\{n\}_q^{a_1}} S_{a_2,...,a_l}(c_2,...,c_l;N;q) \cdot S_{b_1,...,b_m}(d_1,...,d_m;N;q)\\
&\qquad + \sum_{n=1}^{N} \frac{d_1^n}{\{n\}_q^{b_1}} S_{a_1,...,a_l}(c_1,...,c_l;n;q) \cdot S_{b_2,...,b_m}(d_2,...,d_m;n;q)\\
&\qquad - \sum_{n=1}^{N} \frac{(c_1 \cdot d_1)^n}{\{n\}_q^{a_1+b_1}} S_{a_2,...,a_l}(c_2,...,c_l;n;q) \cdot S_{b_2,...,b_m}(d_2,...,d_m;n;q),
\end{aligned}
$$

(5.3)

where additional terms beyond the shuffle-contributions emerge.

Various explicit examples in the case of harmonic sums are given in Refs. [177, 252]. One example is

$$\begin{aligned} S_b(N;q) \cdot S_{a_1,...,a_l}(N;q) &= S_b(N;q) \sqcup\!\sqcup S_{a_1,...,a_l}(N;q) \\ &\quad - S_{b\wedge a_1,a_2,...,a_l}(N;q) - ... - S_{a_1,a_2,...,b\wedge a_l}(N;q) \end{aligned} \tag{5.4}$$

with

$$S_b(N;q) \sqcup\!\sqcup S_{a_1,...,a_l}(N;q) = S_{b,a_1,...,a_l}(N;q) + S_{a_1,b,a_2,...,a_l}(N;q) + ... + S_{a_1,...,a_l,b}(N;q), \tag{5.5}$$

and

$$a \wedge b = (|a| + |b|)\text{sign}(a)\text{sign}(b). \tag{5.6}$$

For the counting of independent iterative integrals and sums, see Refs. [253–257] and Ref. [252].

Let us consider the relations, cf. Ref. [252],

$$S_{1,-1} = -S_{-1,1} + S_1 S_{-1} + S_{-2} \tag{5.7}$$

$$S_{1,-1,-2} = S_{-2} S_{1,-1} + S_{1,3} + S_{3,1} - S_{-2,1,-1} - S_{-1,-2,1} - S_1 S_{-2,-1} + S_{-1} S_{-2,1}, \tag{5.8}$$

$$S_{-1,2,1,-2} = S_{-3,1,-2} + S_{2,-2,-2} + S_{2,1,3} - S_{2,-1,1,-2} - S_{2,1,-2,-1} - S_{2,1,-1,-2} + S_{-1} S_{2,1,-2}, \tag{5.9}$$

$$S_{1,2,3,4} = S_{2,3,5} + S_{2,4,4} + S_{3,3,4} - S_{2,1,3,4} - S_{2,3,1,4} - S_{2,3,4,1} + S_1 S_{2,3,4}, \tag{5.10}$$

where we applied the short-hand notation $S_{\vec{a}}(N;q) \equiv S_{\vec{a}}$. The index pattern implies that the double sum of Eq. (5.7 needs one defining double sum at the r.h.s. For the triple sum Eq. (5.8, two triple sums are needed. For the present pattern in the case of the quadruple sums we used other four-letter relations to shorten the given expression, cf. [252].

We first verify the validity of the shuffle-relations for q-extended harmonic sums at fixed values of N up to a maximal value $N_{\max} = 20$, expanding the q-rational functions. Next we calculate the q-recurrences of both sides of Eqs. (5.7–5.10) and show that they are identical. We obtain the following recurrences for $S_{1,-1}(N;q)$ and for $S_{1,-1,-2}(N;q)$

$$\begin{aligned} &f[n;q]\left(q^{n+2}-1\right)\left(q^{n+3}-1\right) + f[n+1;q]\left(q^{n+3}-1\right)\left(-q^{n+2}-q^{n+3}+q^{n+4}+1\right) \\ &-f[n+2;q]\left(q^{n+3}-3q^{n+4}-q^{2n+6}+q^{2n+7}+q^{2n+8}+1\right) + f[n+3;q]\left(q^{n+4}-1\right)^2 = 0, \end{aligned} \tag{5.11}$$

$$\begin{aligned} &f[n;q]\left(q^{n+4}-1\right)^2\left(-q^{n+2}-q^{n+3}+q^{2n+5}+1\right) + f[n+1;q]\left(q^{n+2}+3q^{n+3}+2\right. \\ &q^{n+4}+q^{3(n+4)}+2q^{n+5}-q^{2(n+5)}-q^{2n+5}-3q^{2n+6}-4q^{2n+7}-q^{2n+8}-2q^{2n+9}+2q^{3n+9} \\ &+3q^{3n+10}+q^{3n+13}+q^{3n+14}-q^{4n+13}-q^{4n+14}+q^{4n+15}-q^{4n+17}-2\Big) \\ &-f[n+2;q]\left((q-1)\left(q^{n+3}+3q^{n+4}-2q^{n+5}-q^{2(n+5)}+q^{3(n+5)}+q^{n+6}-2q^{2n+7}-q^{2n+8}\right.\right. \\ &\left.\left.+2q^{2n+9}-q^{2n+11}+q^{3n+11}-q^{3n+13}+q-2\right)q^{n+3}\right) + f[n+3;q]\left(-3q^{n+4}-4q^{3(n+4)}\right. \\ &\left.+q^{4(n+4)}-5q^{n+5}+8q^{2(n+5)}-5q^{3(n+5)}+q^{4(n+5)}+5q^{2n+8}-q^{2n+9}+2q^{3n+13}-q^{3n+14}\right. \\ &\left.-q^{4n+18}+q^{4n+19}+2\right) - f[n+4;q]\left(q^{n+5}-1\right)^4 = 0. \end{aligned} \tag{5.12}$$

Similar, but much larger, recurrences are obtained for $S_{-2,1,2,-1}(N;q)$ and $S_{1,2,3,4}(N;q)$ and their shuffle-product representations.

Complementary to this, we use the algorithms of the package `Sigma` [194, 195] to reduce the q-sums for general values of N to show the identities. The latter two algorithms can be applied to each individual case of products of nested harmonic sums. Let us illustrate this for Eq. (5.8). One forms the q-sum tower

$$\{S_1, S_{-1}, S_{-2}, S_{-2,-1}, S_{-2,1}, S_{1,-1}, S_{1,3}, S_{3,1}, S_{-2,1,-1}, S_{-1,-2,1}\}, \tag{5.13}$$

over which other sums shall be expressed. By using the `Sigma`-command

$$\begin{aligned}&\texttt{SigmaReduce}[\texttt{qS}[\texttt{q}, 1, -1, -2, \texttt{n}], \texttt{n}, \texttt{Tower} \to \texttt{tower}, \texttt{SimpleSumRepresentation}\\ &\to \texttt{False}, \texttt{qCase} \to \texttt{q}]\end{aligned} \tag{5.14}$$

one obtains the r.h.s. of (5.8), the synonymous relation to the q-free case. More generally, one can start with a tower containing all sums needed to represent any nested sum at a given weight and cannot only prove but even find any identity that is induced by a quasi-shuffle product. The package `Sigma` can be applied to discover the underlying identity.

Let us now turn to generalized harmonic sums in extending the sums in Eqs. (5.7–5.8) by adding the numerator weights

$$\{a, b, c\} \tag{5.15}$$

to the first and second sum and apply the same techniques as for the harmonic sums. We choose

$$\left\{a = 3, \quad b = -\frac{1}{2}, \quad c = \frac{1}{5}\right\} \tag{5.16}$$

as concrete examples. The following recursions are obtained for the respective l.h.s, and r.h.s. of the q extensions of $S_{1,1}(\{a, b\}, n)$ and $S_{1,1,2}(\{a, b, c\}, n)$,

$$\begin{aligned}&9\left(q^{n+1}-1\right)\left(q^{n+2}-1\right)f[n;q] + 3\left(q^{n+2}-1\right)\left((q+1)(2q-3)q^{n+1}+2\right)f[n+1,q]\\ &+\left(10q^{n+3}+(3-2q(q+3))q^{2n+4}-5\right)f[n+2;q] + 2\left(q^{n+3}-1\right)^2 f[n+3;q] = 0,\end{aligned} \tag{5.17}$$

with

$$f[0;q] = 0, \quad f[1;q] = -\frac{3}{2}, \quad f[2;q] = -\frac{3(5+2q(5+q))}{4(1+q)^2}, \tag{5.18}$$

and

$$\begin{aligned}&27\left(q^{n+1}-1\right)\left(q^{n+2}-1\right)\left(q^{n+3}-1\right)^2 f[n;q] + 9\left(q^{n+2}-1\right)\left(q^{n+3}-1\right)\left(\left(\left(q\left(10q^3+2q-1\right)\right.\right.\right.\\ &\left.\left.\left.-3\right)q^{n+3}-20q^3+q+3\right)q^{n+1}+8\right)f[n+1;q] + 3\left(q^{n+3}-1\right)\left(-5(q(4q+5)+6)q^{n+2}\right.\\ &+(2q(2q(18-5(q-1)q)+3)-3)q^{2n+4} + (2q(q(5q(q+1)(2q-3)-1)-3)+3)q^{3n+7}+25\Big)\\ &\times f[n+2;q] + 2\left(q^{n+3}\left(-3(5q(9q+2)-11)q^{n+3}+2(5q(q(7q+6)-3)-6)q^{2n+6}\right.\right.\\ &\left.\left.+\left(3-5q^2(2q(q+3)-3)\right)q^{3n+9}+100q-12\right)-22\right)f[n+3;q]\\ &+20\left(q^{n+4}-1\right)^4 f[n+4;q] = 0,\end{aligned} \tag{5.19}$$

with

$$f[0;q] \;=\; 0, \quad f[1;q] = -\frac{3}{10}, \quad f[2;q] = -\frac{3(5q(q(2q(q+7)+27)+20)+22)}{100(q+1)^4},$$

$$
\begin{aligned}
f[3;q] &= -\frac{3P_4(q)}{1000(q+1)^4\left(q^2+q+1\right)^4}, \\
P_4(q) &= 100q^{12}+1100q^{11}+6050q^{10}+20850q^9+49945q^8+88240q^7+118510q^6. \quad (5.20)
\end{aligned}
$$

For the shuffle relations of the iterated integrals, Eq. (5.2), we consider the formal series expansion around $x = 0$ for the left and the right-hand sides, see Eq. (1.3) or its extensions being modulated by a finite number of powers in $\ln(x)$,

$$
\sum_{n=0}^{\infty} f_l[n]x^n = \sum_{n=0}^{\infty} f_r[n]x^n. \quad (5.21)
$$

Both $f_l[n]$ and $f_r[n]$ are sum-product structures, which can be q-extended as described before. The identity $f_l[n] = f_r[n]$ implies the identity $f_l[n;q] = f_r[n;q]$ of the q-extensions. Therefore, the q-extension preserves the shuffle product. Similarly as above, one may also use the package `Sigma` to discover the underlying identity.

Shuffle-algebras are Hopf-algebras [258–261], with the product implied by the shuffle product, cf. Ref. [262].

6 Conclusions

Perturbative calculations in quantum field-theories are based on Feynman integrals, which describe all contributions up to a given power in the coupling constant. In the case of single or double-scale integrals, the respective integrals can be carried out analytically and are given as functions in special function spaces either as iterated integrals or nested sums. This applies to the iterated integrals as polylogarithms, Nielsen integrals, harmonic polylogarithms, generalized harmonic polylogarithms, cyclotomic harmonic polylogarithms, iterated integrals implied by quadratic forms, and iterated integrals over square-root valued letters, [158–175]. For the nested sums we have considered the q-extensions of the harmonic sums, generalized harmonic sums, cyclotomic harmonic sums, nested sums implied by quadratic forms, and nested sums weighted by central binomial coefficients [171–177]. We considered the classes of iterative integrals obeying first order factorizing differential equations and nested sums obeying first order factorizing difference equations.

Like also the case in other special functions, cf. Refs. [2–17], one may construct the associated q-extension for these functions. From the quantum field theoretic point of view, the q-extension is implied by the q-deformation of the commutation relation, Eq. (1.2), and the associated dynamical equations.

The different spaces of the q-extended nested sums are determined by recursions of finite order and degree, depending on the deformation parameter q. Likewise, the spaces of iterated integrals are defined by q-differential and q-shift relations of finite order and degree. For the single sums, the polylogarithms and Nielsen integrals, closed form q-extensions have been derived. For the higher sum- and function spaces algorithms exist to derive the q-extension in the respective individual cases. In the present approach the starting point to derive the q-extensions is the Taylor expansion of the non q-deformed functions at $x = 0$, cf. Eq. (1.3). For the central functions $f[n;q]$ a q-recursion can be obtained by guessing methods. One may also consider q-extensions by expanding around another value as $x = x_0$ and find overlapping representations to map out the considered region of x, beyond the convergence radius of the q-expansion around $x = 0$. The package `Sigma` [194,195] enables one to solve all derived q-recursions for the functions

$f[n;q]$ to obtain the respective initial representation. We used this as an essential check of these relations.

Unlike the case for the μ-deformation, Ref. [178], in the case of iterated integrals based on square-root valued letters, their q-extension remains in the same function class. Both the q-extended nested sums and iterated integrals form (quasi-)shuffle algebras and therefore by the shuffle product Hopf algebras, cf. Ref. [262].

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