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Orthopositronium lifetime at $\mathcal{O}(\alpha)$ and $\mathcal{O}(\alpha^3 \ln \alpha)$ in closed form

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Abstract

Recently, the $\mathcal{O}(\alpha)$ and $\mathcal{O}(\alpha^3 \ln \alpha)$ radiative corrections to the orthopositronium lifetime have been presented in closed analytical form, in terms of basic irrational numbers that can be evaluated numerically to arbitrary precision [Phys. Rev. Lett. **101**, 193401 (2008)]. Here, we present the details of this calculation and reveal the nature of these new constants. We also list explicit transformation formulas for generalized polylogarithms of weight four, which may be useful for other applications.

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I. INTRODUCTION

Positronium (Ps), the electron-positron bound state, was discovered experimentally in 1951 [1]. Since that time a lot of attention has been paid to the determination of its properties, including lifetime, decay modes, and spectroscopy. The experimental and theoretical accuracies achieved by now being quite high, there is little doubt that quantum electrodynamics (QED) is the only interaction in this system. In fact, thanks to the smallness of the electron mass m relative to typical hadronic mass scales, its theoretical description is not plagued by strong-interaction uncertainties and its properties, such as decay widths and energy levels, can be calculated perturbatively in non-relativistic QED (NRQED) [2], as expansions in Sommerfeld's fine-structure constant α, with very high precision.

Ps comes in two ground states, $^1S_0$ parapositronium (p-Ps) and $^3S_1$ orthopositronium (o-Ps), which decay to two and three photons, respectively. Here we are concerned with the lifetime of o-Ps, which has been the subject of a vast number of experimental and theoretical investigations. Its first measurement [3] was performed later in the year 1951 and agreed well with its lowest-order (LO) prediction of 1949 [4]. Its first precision measurement [5], of 1968, had to wait 9 years for the first correct one-loop calculation [6], which came two decades after the analogous calculation for p-Ps [7] being considerably simpler owing to the two-body final state. In the year 1987, the Ann Arbor group [8] published a measurement that exceeded the best theoretical prediction available then by more than 8 experimental standard deviations. This so-called o-Ps lifetime puzzle triggered an avalanche of both experimental and theoretical activities, which eventually resulted in what now appears to be the resolution of this puzzle. In fact, the 2003 measurements at Ann Arbor [9] and Tokyo [10],

$$\begin{aligned} \Gamma(\text{Ann Arbor}) &= 7.0404(10\ \text{stat.})(8\ \text{syst.})\ \mu s^{-1}, \\ \Gamma(\text{Tokyo}) &= 7.0396(12\ \text{stat.})(11\ \text{syst.})\ \mu s^{-1}, \end{aligned} \tag{1}$$

agree mutually and with the present theoretical prediction,

$$\Gamma(\text{theory}) = 7.039979(11)\ \mu s^{-1}. \tag{2}$$

The latter is evaluated from

$$\Gamma(\text{theory}) = \Gamma_0 \left[1 + A\frac{\alpha}{\pi} + \frac{\alpha^2}{3}\ln\alpha + B\left(\frac{\alpha}{\pi}\right)^2 - \frac{3\alpha^3}{2\pi}\ln^2\alpha + C\frac{\alpha^3}{\pi}\ln\alpha\right], \tag{3}$$

where [4]

$$\Gamma_0 = \frac{2}{9}(\pi^2 - 9)\frac{m\alpha^6}{\pi} \tag{4}$$

is the LO result. The leading logarithmically enhanced $\mathcal{O}(\alpha^2 \ln \alpha)$ and $\mathcal{O}(\alpha^3 \ln^2 \alpha)$ terms were found in Refs. [11, 12] and Ref. [13], respectively. The coefficients $A = -10.286606(10)$ [6, 11, 14, 15, 16], $B = 45.06(26)$ [15], and $C = -5.51702455(23)$ [17] were evaluated numerically in a series of papers. Comprehensive reviews of the experimental and theoretical status of Ps may be found in Refs. [18, 19].

We note in passing that high-precision tests make Ps also a useful probe of new physics beyond he standard model. At present, there is strong interest in models with extra dimensions [20], which may provide a solution of the gauge hierarchy problem [21] (see Ref. [22] for a review). Some time ago, a peculiar feature of matter in brane world was observed in Ref. [23], where it was shown that massive particles initially located on our brane may leave the brane and disappear into extra dimensions. The experimental signature of this effect is the disappearance of a particle from our world, *i.e.* its invisible decay. The case of the electromagnetic field propagating in the Randall–Sundrum type of metric in the presence of extra compact dimensions [24, 25] was considered in Ref. [25], where it was shown that the transition rate of a virtual photon into extra dimensions is non-zero. This effect could result in the disappearance of a neutral system. In the case of o-Ps, such estimations for the invisible decay branching fraction $B(o\text{-Ps} \to \mathit{invisible})$ [19, 26] range just one order of magnitude below the presently best experimental upper bound of 4.3×10^{-7} at 90% confidence level established by Badertscher *et al.* [27]. Thus, this decay is of great interest for the possible observation of effects due to extra dimensions.

In order to reduce the theoretical uncertainty in the o-Ps total decay width $\Gamma(\text{theory})$, it is indispensable to increase the precision in the coefficients A, B, and C in Eq. (3). This is most efficiently done by avoiding numerical integrations altogether, *i.e.* by establishing the analytic forms of these coefficients. The case of B is beyond the scope of presently available technology, since it involves two-loop five-point functions to be integrated over the three-particle phase space. In the following, we thus concentrate on A and C. The quest for an analytic expression for A has a long history. About 25 years ago, some of the simpler contributions to A, due to self-energy and outer and inner vertex corrections, were obtained analytically [28], but further progress then soon came to a grinding halt. In our recent Letter [29], this task was completed for A as a whole. The purpose of the present paper is to explain the most important technical details of this calculation and to collect mathematical identities that may be useful for similar calculations.

An analytic expression for C is then simply obtained from that for A through the relationship [17]

$$C = \frac{A}{3} - \frac{229}{30} + 8 \ln 2, \tag{5}$$

which may be understood qualitatively by observing that the $\mathcal{O}(\alpha^3 \ln \alpha)$ correction in Eq. (3) receives a contribution from the interference of the relativistic $\mathcal{O}(\alpha)$ term from

the hard scale with non-relativistic $\mathcal{O}(\alpha^2 \ln \alpha)$ terms from softer scales.

The structure of this paper is as follows. Section II contains the well-known integral representation of the o-Ps total decay width as given in Ref. [16]. In Sec. III, we show how to transform the contributing integrals to forms appropriate for analytic evaluation, which is carried out for the most complicated integrals, which are plagued by singularities, in Sec. IV. More examples are studied in Sec. V. The final results for the coefficients A and C are presented in Sec. VI. Section VII contains a summary. In Appendix A, we present the analytic results for all parts of the integral representation given in Sec. II. Appendix B contains useful representations of the ψ function and the expansion of the Γ function about half-integer-valued arguments. In Appendix C, transformation formulas for generalized polylogarithms of weight four with different arguments are collected.

II. DEFINITIONS AND NOTATIONS

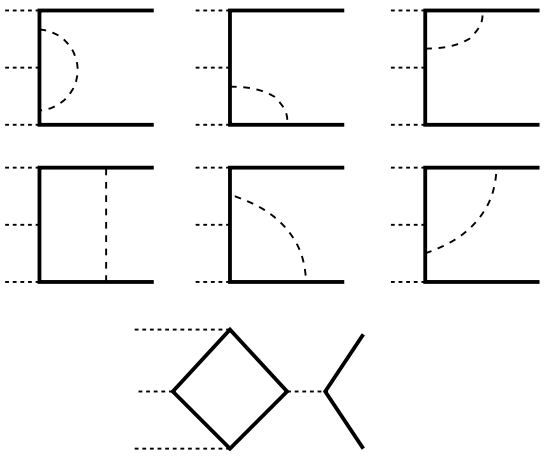

FIG. 1: Feynman diagrams contributing to the total decay width of o-Ps at $\mathcal{O}(\alpha)$. Self-energy diagrams are not shown. Dashed and solid lines represent photons and electrons, respectively.

The $\mathcal{O}(\alpha)$ contribution in Eq. (3), $\Gamma_1 = \Gamma_0 A \alpha/\pi$, is due to the Feynman diagrams where a virtual photon is attached in all possible ways to the tree-level diagrams, with three real photons linked to an open electron line, and the electron box diagrams with an e^+e^- annihilation vertex connected to one of the photons being virtual (see Fig. 1). Taking the interference with the tree-level diagrams, imposing e^+e^- threshold kinematics, and performing the loop and angular integrations, one obtains the two-dimensional integral

representation [16]

$$\Gamma_1 = \frac{m\alpha^7}{36\pi^2} \int_0^1 \frac{dx_1}{x_1} \frac{dx_2}{x_2} \frac{dx_3}{x_3} \delta(2 - x_1 - x_2 - x_3)[F(x_1, x_3) + \text{perm.}], \tag{6}$$

where x_i, with $0 \le x_i \le 1$, is the energy of photon i in the o-Ps rest frame normalized to its maximum value, the delta function ensures energy conservation, and "perm." stands for the other five permutations of x_1, x_2, x_3. The function $F(x_1, x_3)$ is given by

$$F(x_1, x_3) = g_0(x_1, x_3) + \sum_{i=1}^{5} g_i(x_1, x_3) h_i(x_1) + \sum_{i=6}^{7} g_i(x_1, x_3) h_i(x_1, x_3), \tag{7}$$

where $g_i(x_1, x_3)$ are ratios of polynomials, which are listed in Eqs. (A5a)–(A5h) of Ref. [16], and

$$h_1(x_1) = \ln(2x_1), \qquad h_2(x_1) = \sqrt{\frac{x_1}{\overline{x}_1}}\,\theta_1, \qquad h_3(x_1) = \frac{1}{2x_1}[\zeta(2) - \mathrm{Li}_2(1 - 2x_1)],$$
$$h_4(x_1) = \frac{1}{4x_1}[3\zeta(2) - 2\theta_1^2], \qquad h_5(x_1) = \frac{1}{2\overline{x}_1}\theta_1^2, \tag{8}$$

$$h_6(x_1, x_3) = \frac{1}{\sqrt{x_1 \overline{x}_1 x_3 \overline{x}_3}} \left[\mathrm{Li}_2\left(r_A^+, \overline{\theta}_1\right) - \mathrm{Li}_2\left(r_A^-, \overline{\theta}_1\right)\right], \tag{9}$$

$$h_7(x_1, x_3) = \frac{1}{2\sqrt{x_1 \overline{x}_1 x_3 \overline{x}_3}} \left[2\,\mathrm{Li}_2(r_B^+, \theta_1) - 2\,\mathrm{Li}_2(r_B^-, \theta_1) - \mathrm{Li}_2(r_C^+, 0) + \mathrm{Li}_2(r_C^-, 0)\right], \tag{10}$$

where $\overline{x}_i = 1 - x_i$ and

$$\theta_1 = \arctan\sqrt{\frac{\overline{x}_1}{x_1}}, \qquad \overline{\theta}_1 = \arctan\sqrt{\frac{x_1}{\overline{x}_1}}, \qquad p_A = \sqrt{\frac{x_1 \overline{x}_3}{\overline{x}_1 x_3}}, \qquad p_B = \sqrt{\frac{\overline{x}_1 \overline{x}_3}{x_1 x_3}},$$
$$r_A^\pm = \sqrt{\overline{x}_1}\,(1 \pm p_A), \qquad r_B^\pm = \sqrt{x_1}\,(1 \pm p_B), \qquad r_C^\pm = \frac{r_B^\pm}{\sqrt{x_1}}. \tag{11}$$

Here, $\zeta(2) = \pi^2/6$ and

$$\mathrm{Li}_2(r, \theta) = -\frac{1}{2} \int_0^1 \frac{dt}{t} \ln(1 - 2rt\cos\theta + r^2 t^2) \tag{12}$$

is the real part of the dilogarithm [see line below Eq. (32)] of complex argument $z = re^{i\theta}$ [30]. Since we are dealing here with a single-scale problem, Eq. (6) yields just a number.

Although Bose symmetry is manifest in Eq. (6), its evaluation is complicated by the fact that, for a given order of integration, individual permutations yield divergent integrals, which have to cancel in their combination. In order to avoid such a proliferation of terms,

we introduce an infinitesimal regularization parameter δ in such a way that the symmetry under $x_i \leftrightarrow x_j$ for any pair $i \neq j$ is retained. In this way, Eq. (6) collapses to

$$\Gamma_1 = \frac{m\alpha^7}{6\pi^2} \int\limits_{2\delta}^{1-\delta} dx_1 \int\limits_{1-x_1+\delta}^{1-\delta} \frac{dx_2}{x_1 x_2 x_3} F(x_1, x_3), \tag{13}$$

where $x_3 = 2 - x_1 - x_2$. Note that we may now exploit the freedom to choose any pair of variables x_i and x_j $(i \neq j)$ as the arguments of F and as the integration variables.

III. INTEGRAL REPRESENTATIONS OF DILOGARITHMIC FUNCTIONS

Obviously, the functions $h_6(x_1, x_3)$ and $h_7(x_1, x_3)$ in Eqs. (9) and (10), respectively, give the most complicated contributions to Γ_1. In order to perform integrations involving these terms, it is useful to apply the integral representation of Eq. (12) to $\mathrm{Li}_2(r_A^{\pm}, \overline{\theta}_1)$, $\mathrm{Li}_2(r_B^{\pm}, \theta_1)$, and $\mathrm{Li}_2(r_C^{\pm}, 0)$. Let us first consider $\mathrm{Li}_2(r_B^{+}, \theta_1)$. We see from Eq. (11) that $\cos\theta_1 = \sqrt{x_1}$ and thus

$$\mathrm{Li}_2(r_B^{+}, \theta_1) = -\frac{1}{2} \int\limits_{0}^{1+p_B} \frac{dt_1}{t_1} \ln[1 - x_1 t_1 (2 - t_1)], \tag{14}$$

where $t_1 = (1 + p_B)t$. Then, the term $D_1 = \mathrm{Li}_2(r_B^{+}, \theta_1) - \mathrm{Li}_2(r_B^{-}, \theta_1)$ on the r.h.s. of Eq. (10), after the change $t_2 = t_1 - 1$, can be rewritten as

$$D_1 = -\frac{1}{2} \int\limits_{-p_B}^{p_B} \frac{dt_2}{1 + t_2} \ln[1 - x_1 (1 - t_2^2)]. \tag{15}$$

Finally, substituting $t_2 = p_B \sqrt{t}$, we obtain

$$D_1 = -\frac{1}{2} \sqrt{x_1 \overline{x}_1 x_3 \overline{x}_3} \int\limits_{0}^{1} \frac{dt}{\sqrt{t}(x_1 x_3 - \overline{x}_1 \overline{x}_3 t)} [\ln \overline{x}_1 - \ln x_3 + \ln(x_3 + \overline{x}_3 t)]. \tag{16}$$

The residual term on the r.h.s. of Eq. (10), $D_2 = \mathrm{Li}_2(r_C^{+}, 0) - \mathrm{Li}_2(r_C^{-}, 0)$, can be transformed in the same way yielding

$$D_2 = -\frac{1}{2} \sqrt{x_1 \overline{x}_1 x_3 \overline{x}_3} \int\limits_{0}^{1} \frac{dt}{\sqrt{t}(x_1 x_3 - \overline{x}_1 \overline{x}_3 t)} [\ln(\overline{x}_1 \overline{x}_3) - \ln(x_1 x_3) + \ln t]. \tag{17}$$

We thus obtain the following integral representation for $h_7(x_1, x_3)$ [48]:

$$h_7(x_1,x_3) = -\frac{1}{4}\int_0^1 \frac{dt}{\sqrt{t}\,(x_1x_3 - \overline{x}_1\overline{x}_3 t)}\left[\ln\frac{\overline{x}_1 x_1}{x_3\overline{x}_3} + 2\ln(x_3+\overline{x}_3 t) - \ln t\right]. \tag{18}$$

Exploiting the $x_1 \leftrightarrow x_3$ symmetry of the coefficient $g_7(x_1, x_3)$ multiplying $h_7(x_1, x_3)$, Eq. (18) can be effectively replaced by

$$\tilde{h}_7(x_1,x_3) = -\frac{1}{4}\int_0^1 \frac{dt}{\sqrt{t}\,(x_1x_3 - \overline{x}_1\overline{x}_3 t)}[2\ln(x_3+\overline{x}_3 t) - \ln t]. \tag{19}$$

Next, this expression, multiplied by $g_7(x_1, x_3)$, is to be integrated over x_1, x_3, and t. Observing that the logarithmic terms in Eq. (19) are independent of x_1, we first integrate over x_1 (for a similar approach, see Ref. [31]). In order to avoid the appearance of complicated functions in the intermediate results, the integration over t in Eq. (19) is performed last.

Using the same technique, we obtain the following representation for the function $h_6(x_1, x_3)$:

$$\tilde{h}_6(x_1,x_3) = -\frac{1}{2}\int_0^1 \frac{dt}{\sqrt{t}(\overline{x}_1x_3 - x_1\overline{x}_3 t)}[\ln x_1 - \ln x_3 + \ln(x_3+\overline{x}_3 t)], \tag{20}$$

in which the part proportional to $\ln x_1$ and the complementary one are first integrated over x_3 and x_1, respectively. The t integration is again performed last.

In Secs. IV and V, we discuss in more details how these integrations can be performed.

IV. EVALUATION OF CONTRIBUTIONS WITH h_6 AND h_7

We now discuss the evaluation of the most complicated integrals, namely those involving the functions $h_6(x_1, x_3)$ and $h_7(x_1, x_3)$. We denote the corresponding integrated expressions as I_6 and I_7, respectively. They are both singular for $\delta \to 0$, so that the regularization of Eq. (13) is indispensable.

Let us first consider the contribution of the coefficient $g_7(x_1, x_3)$ without the function $h_7(x_1, x_3)$. It can be decomposed into two parts, as

$$\tilde{g}_7(x_1,x_3) = \frac{g_7(x_1,x_3)}{x_1x_3(2-x_1-x_3)} = \tilde{g}_7^{\rm sing}(x_1,x_3) + \tilde{g}_7^{\rm reg}(x_1,x_3), \tag{21}$$

where

$$\tilde{g}_7^{\rm sing}(x_1,x_3) = \frac{3x_3(1-x_3)}{2-x_1-x_3} \tag{22}$$

gives rise to the singularity upon integration over x_1 and x_3, while

$$\tilde{g}_7^{\rm reg}(x_1,x_3) = \frac{18}{x_3} - 3 + 9x_3 + \left(\frac{2}{x_3} - 10\right) x_1 + \left(\frac{4}{2-x_3} - \frac{8}{x_3} + 10 + 2x_3\right) \frac{1}{x_1} + \left(-\frac{52}{2-x_3} - \frac{12}{x_3} + 66 - 44x_3 + 11x_3^2\right) \frac{1}{2-x_1-x_3} \tag{23}$$

remains finite, so that the limit $\delta \to 0$ can be taken. A similar decomposition can be made also for $g_6(x_1,x_3)$. Specifically, performing the integrations over x_1 and x_3 and taking the limit $\delta \to 0$, we have

$$6 \int\limits_{2\delta}^{1-\delta} dx_1 \int\limits_{1-x_1+\delta}^{1-\delta} dx_3\, \tilde{g}_7^{\rm sing}(x_1,x_3) = 3\ln\delta + \frac{5}{2} + \mathcal{O}(\delta),$$
$$6 \int\limits_{2\delta}^{1-\delta} dx_1 \int\limits_{1-x_1+\delta}^{1-\delta} dx_3\, \tilde{g}_7^{\rm reg}(x_1,x_3) = \frac{1240}{3} - 264\zeta(2) + \mathcal{O}(\delta). \tag{24}$$

Observing that the presence of the functions $h_6(x_1,x_3)$ and $h_7(x_1,x_3)$ does not change the singularity structure of the integrals over the variables x_3, x_1, and t in this order, the decomposition of Eq. (21) leads to

$$I_i = I_i^{\rm sing} + I_i^{\rm reg}, \qquad I_i^{\rm sing,\,reg} = 6 \int\limits_{2\delta}^{1-\delta} dx_3 \int\limits_{1-x_3+\delta}^{1-\delta} dx_1\, \tilde{g}_i^{\rm sing,\,reg}(x_1,x_3) h_i(x_1,x_3), \tag{25}$$

with $i = 6, 7$.

Our evaluation yields

$$I_6^{\rm sing} = 9\ln\delta + 45 + \frac{9}{2}\zeta_2 - \frac{63}{2}\zeta_3 + \mathcal{O}(\delta), \tag{26}$$
$$I_6^{\rm reg} = -\frac{422}{3} + \zeta_2\left(\frac{1877}{3} - 1590 l_2 - 288 l_2^2\right) + \frac{2719}{2}\zeta_3 - 24 l_2^4 + \frac{7677}{16}\zeta_4 - 576\,{\rm Li}_4\left(\frac{1}{2}\right) + \frac{35}{\sqrt{2}} G_3 + \mathcal{O}(\delta), \tag{27}$$
$$I_7^{\rm sing} = -9\ln\delta - 36 - \frac{27}{2}\zeta_2 + \frac{63}{2}\zeta_3 + \mathcal{O}(\delta), \tag{28}$$
$$I_7^{\rm reg} = 297 + \zeta_2\Big(-222 + 486 l_2\Big) - \frac{567}{2}\zeta_3 + \frac{315}{16}\zeta_4 + \frac{24}{\sqrt{2}} G_3 + \mathcal{O}(\delta), \tag{29}$$

where [49]

$$G_3 = 12\zeta_2 l_2 - l_2^3 - 39\zeta_2 l_R - 3 l_2^2 l_R + l_R^3 - \frac{21}{4}\zeta_3 + 48\,{\rm Li}_3\left(\frac{1}{\sqrt{2}}\right) + 3\,{\rm Re}\left[{\rm Li}_3\left(\frac{1-\sqrt{2}}{2}\right) - {\rm Li}_3\left(\frac{1+\sqrt{2}}{2}\right)\right]. \tag{30}$$

As can be seen from Eqs. (26) and (28), $\ln\delta$ cancels in the sum $I_6 + I_7$. Here and in the following, we use the short-hand notations

$$l_2 = \ln 2, \qquad l_3 = \ln 3, \qquad l_R = \ln\left(1+\sqrt{2}\right). \tag{31}$$

Furthermore,

$$\mathrm{S}_{n,p}(x) = \frac{(-1)^{n+p-1}}{(n-1)!p!}\int\limits_0^1 \frac{dt}{t}\,\ln^p(1-tx)\,\ln^{n-1}t \tag{32}$$

is the generalized Nielsen polylogarithm, $\mathrm{Li}_n(x) = \mathrm{S}_{n-1,1}(x)$ the polylogarithm of order n, and $\zeta_n = \zeta(n) = \mathrm{Li}_n(1)$, with $\zeta(x)$ being Riemann's zeta function [30, 32].

The result of Eq. (30), which is the most complicated part arising from the terms with $i = 6$ and 7 in Eq. (7), assumes a rather simple form when written as an infinite series,

$$\frac{\sqrt{2}}{3}G_3 = 14\zeta_3 - 24\zeta_2 l_2 - \frac{1}{2}\sum_{n=1}^{\infty}\frac{\Gamma^2(n)}{\Gamma(2n)}4^n\left[\psi'\left(\frac{n+2}{2}\right) - \psi'\left(\frac{n+1}{2}\right)\right], \tag{33}$$

where $\psi^{(m)}(n)$ is the $(m+1)$-th logarithmic derivative of the Γ function, $\Gamma(x) = \int_0^\infty dt\,\mathrm{e}^{-t}t^{x-1}$. We can now apply the well-known relations for Γ and ψ functions,

$$\frac{\Gamma^2(n)}{2\Gamma(2n)} = \frac{1}{\binom{2n}{n}}\frac{1}{n}, \tag{34}$$

$$\psi'\left(\frac{n+2}{2}\right) - \psi'\left(\frac{n+1}{2}\right) = (-1)^n 4\left[-\frac{1}{2}\zeta_2 - S_{-2}(n)\right], \tag{35}$$

where

$$S_{\pm m}(n) = \sum_{j=1}^{n}\frac{(\pm 1)^j}{j^m} \tag{36}$$

is the harmonic sum. Using Eqs. (34) and (35), the constant G_3 is rewritten in terms of so-called inverse central binomial sums, *i.e.* sums of the form

$$\sum_{n=1}^{\infty}\frac{z^n}{\binom{2n}{n}}\phi(n), \tag{37}$$

where $\phi(n)$ is some combination of harmonic sums and factors like $1/n$, and z is some number. Sums of such type were studied in great detail in Refs. [33, 34, 35, 36].

It is known that, for the series in Eq. (37), there exists a nonlinear transformation,

$$y = \frac{\sqrt{z-4}-\sqrt{z}}{\sqrt{z-4}+\sqrt{z}}, \tag{38}$$

which leads to great simplifications in many cases. The series in the new variable y does not have a binomial coefficient and can be summed, yielding expressions involving generalized polylogarithms $\mathrm{S}_{n,p}(y)$.

Now we can explain the appearance of the prefactor $1/\sqrt{2}$ in front of G_3 in Eqs. (27) and (29). Such a prefactor has not appeared in single-scale calculations so far. The point is that all inverse binomial series involving products of the factor $1/n$ and some function $f(n)$ that is a combination of the ψ function and its derivatives have the form (see, for example, Ref. [36])

$$\sum_{n=1}^{\infty} \frac{\Gamma^2(n)}{\Gamma(2n)} z^n f(n) = 2 \sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{z^n}{n} f(n) = \frac{1-y}{1+y} F(y), \tag{39}$$

where $F(y)$ is some combination of generalized polylogarithms and y is defined by Eq. (38). Note that Eq. (35) contains the binomial sum $S_{-2}(n)$, which is related to the basic one, $S_{-2}(n-1)$, via

$$S_{-2}(n) = S_{-2}(n-1) + \frac{(-1)^n}{n^2}. \tag{40}$$

Thus, the last term on the r.h.s. of Eq. (40) leads to $z = 4$ in Eq. (33), which translates to $y = -1$ via Eq. (38). This term then cancels the term $14\zeta_3 - 24\zeta_2 l_2$ on the r.h.s. of Eq. (33). For the term $-\zeta_2/2 - S_{-2}(n-1)$ on the r.h.s. of Eq. (35), we have $z = -4$ so that the variable y from Eq. (38) assumes the value

$$r = \frac{\sqrt{2}-1}{\sqrt{2}+1}. \tag{41}$$

This explains the appearance of the factor $1/\sqrt{2}$ in Eqs. (27) and (29), since $(1-y)/(1+y) = 1/\sqrt{2}$.

Finally, we can rewrite Eq. (30) as

$$G_3 = 21\zeta_2 l_r - \frac{1}{12} l_r^3 - 5 l_r \,\mathrm{Li}_2(r) + 5\,\mathrm{Li}_3(r) - 50\,\mathrm{S}_{1,2}(r) + 4\,\mathrm{S}_{1,2}(r^2) + 34\zeta_3, \tag{42}$$

where $l_r = \ln r$.

V. EVALUATING INTEGRALS FROM SERIES

Let us now consider several typical integrals that arise upon the first integration [50]. Our first example of the remaining two-fold integrals reads

$$I_{\pm} = \int_0^1 \frac{dt}{t} \int_0^1 \frac{dx}{x} \ln[1 \mp 4t(1-t)(1-x)] \ln(1-x). \tag{43}$$

Direct integration over t or x would lead to rather complicated functions in the remaining variable. Instead, we Taylor expand the first logarithm using $\ln(1-q) = -\sum_{n=1}^{\infty} q^n/n$ to obtain

$$I_{\pm} = -\sum_{n=1}^{\infty} \frac{(\pm 4)^n}{n} \int\limits_0^1 \frac{dt}{t}[t(1-t)]^n \int\limits_0^1 \frac{dx}{x}(1-x)^n \ln(1-x). \tag{44}$$

Now, the two integrals are separated and can be solved in terms of Euler's Γ function. Using

$$\int\limits_0^1 \frac{dx}{x}(1-x)^n \ln(1-x) = -\psi'(n+1), \tag{45}$$

we finally have

$$I_{\pm} = \sum_{n=1}^{\infty} \frac{\Gamma^2(n)}{\Gamma(2n)} \frac{(\pm 4)^n}{2n} \psi'(n+1) = \sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{(\pm 4)^n}{n^2} \left[\zeta_2 - S_2(n)\right]. \tag{46}$$

Clearly, in the cases of I_+ and I_-, the argument z in Eq. (37) is equal to 4 and -4, respectively.

The case of I_+ is simpler and leads to a smaller number of constants. Indeed, we can use the results of Refs. [35, 36] to obtain

$$\begin{aligned}
&\sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{4^n}{n^2} = 3\zeta_2, \qquad \sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{4^n}{n^2} S_2(n-1) = \frac{15}{4}\zeta_4, \\
&\sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{4^n}{n^4} = 4\zeta_2 l_2^2 + \frac{l_2^4}{3} + 8\,\mathrm{Li}_4\left(\frac{1}{2}\right) - \frac{19}{4}\zeta_4,
\end{aligned} \tag{47}$$

and so on. According to Ref. [36], after transformation to the variable y of Eq. (38), we arrive at polylogarithms of argument -1, which are expressed in terms of alternating and non-alternating Euler–Zagier sums, such as $\zeta(\pm a) = \sum_{n=1}^{\infty} (\pm 1)^n/n^a$, $\zeta(\pm a, \pm b) = \sum_{m=1}^{\infty} \sum_{n=m+1}^{\infty} (\pm 1)^n (\pm 1)^m/(n^a m^b)$, etc.

Let us now turn to the case of I_- in Eq. (46). The argument $z = -4$ gives $y = r$ and leads to a new type of constants. Again using formulas from Ref. [36], we have

$$\begin{aligned}
&\sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{(-4)^n}{n^2} = -\frac{1}{2} l_r^2, \qquad \sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{(-4)^n}{n^2} S_2(n-1) = \frac{1}{24} l_r^4, \\
&\sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{(-4)^n}{n^4} = -\frac{2}{3} l_r^3 - \frac{1}{8} l_r^4 + 4\,\mathrm{S}_{2,2}(r) - 4\,\mathrm{Li}_4(r) + 4 l_2 [\mathrm{Li}_3(r) - \zeta_3] \\
&\qquad\qquad + 4 l_r [\mathrm{Li}_3(r) - \mathrm{S}_{1,2}(r) - l_2\,\mathrm{Li}_2(r)] - l_r^2 [2\,\mathrm{Li}_2(r) + l_2^2].
\end{aligned} \tag{48}$$

With the help of the relations listed in Appendix C, $I_\pm$ can be alternatively expressed as

$$I_+ = -4\zeta_2 l_2^2 - \frac{l_2^4}{3} + \frac{17}{2}\zeta_4 - 8\,\mathrm{Li}_4\left(\frac{1}{2}\right), \tag{49}$$

$$\begin{aligned} I_- = {} & \zeta_4 - \frac{1}{3}l_2^4 + 2l_2^2\zeta_2 + 5l_2^2 l_R^2 - \frac{19}{2}l_R^2\zeta_2 - \frac{5}{3}l_R^4 \\ & - 4l_R\,\mathrm{Re}\left[\mathrm{Li}_3\left(\frac{1-\sqrt{2}}{2}\right) - \mathrm{Li}_3\left(\frac{1+\sqrt{2}}{2}\right)\right] \\ & - 4\,\mathrm{Re}\left[\mathrm{Li}_4\left(\frac{1-\sqrt{2}}{2}\right) + \mathrm{Li}_4\left(\frac{1+\sqrt{2}}{2}\right)\right]. \end{aligned} \tag{50}$$

It has been observed empirically that, at weight four, the terms that are not expressed through the usual Riemann zeta function $\zeta(a)$ often come in the combination $b_4 = l_2^2(l_2^2/3 - 2\zeta_2) + 8\,\mathrm{Li}_4(1/2)$ introduced by Broadhurst in Ref. [38]. Examples include the three-loop QCD correction to the electroweak ρ parameter [39], the electron anomalous magnetic moment at three loops [40], critical exponents in high orders of perturbation theory [41], the heavy-quark contribution to the vacuum polarization function at four loops in QCD [42], and the matching conditions for the strong-coupling constant at five loops [43]. Our result for I_+ in Eq. (49) exhibits a violation of this empirical observation. In fact, the non-zeta terms form some different combination there.

Another class of typical integrals yields sums involving ψ functions of half-integer arguments (see Appendix B), *e.g.*

$$\begin{aligned} J_\pm &= \int_0^1 \frac{dt}{t} \int_0^1 dx \frac{\ln[1 \mp 4t(1-t)(1-x)]\ln(1-x)}{x-2} \\ &= \sum_{n=1}^{\infty} \frac{(\pm 4)^n}{8n} \frac{\Gamma^2(n)}{\Gamma(2n)} \left[\psi'\left(\frac{n+2}{2}\right) - \psi'\left(\frac{n+1}{2}\right)\right] \\ &= \sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}} \frac{(\mp 4)^n}{n^2} \left[-\frac{1}{2}\zeta_2 - S_{-2}(n-1) - \frac{(-1)^n}{n^2}\right]. \end{aligned} \tag{51}$$

Following a similar strategy as above and using formulas from Sec. IV, we may express

$J_\pm$ in terms of known irrational constants, as

$$\begin{aligned}
J_+ &= -\frac{5}{2}\zeta_2 l_2^2 + \frac{17}{48} l_2^4 + \frac{21}{4}\zeta_4 - 9\zeta_2 l_2 l_R + \frac{19}{2}\zeta_2 l_R^2 + \frac{5}{12} l_R^4 \\
&\quad - 9\,\mathrm{Re}\left[\mathrm{Li}_4\left(\frac{1-\sqrt{2}}{2}\right) + \mathrm{Li}_4\left(\frac{1+\sqrt{2}}{2}\right)\right] + 4\left[\mathrm{Li}_4\left(\frac{2-\sqrt{2}}{4}\right) + \mathrm{Li}_4\left(\frac{2+\sqrt{2}}{4}\right)\right] \\
&= -\frac{5}{2}\zeta_2 l_2^2 + \frac{17}{48} l_2^4 + \frac{21}{4}\zeta_4 - G_4, \\
J_- &= \frac{1}{2}\zeta_2 l_2^2 - \frac{49}{48} l_2^4 - \zeta_4 + 6\,\mathrm{Li}_4\left(\frac{1}{2}\right) + l_R^2\left(3 l_2^2 - \frac{11}{2}\zeta_2\right) - \frac{7}{4} l_R^4 \\
&\quad + l_R\left\{\frac{1}{3} l_2^3 + 5\zeta_2 l_2 + \frac{7}{4}\zeta_3 - 16\,\mathrm{Li}_3\left(\frac{1}{\sqrt{2}}\right) - 5\,\mathrm{Re}\left[\mathrm{Li}_3\left(\frac{1-\sqrt{2}}{2}\right) - \mathrm{Li}_3\left(\frac{1+\sqrt{2}}{2}\right)\right]\right\} \\
&\quad + 5\,\mathrm{Re}\left[\mathrm{Li}_4\left(\frac{1-\sqrt{2}}{2}\right) + \mathrm{Li}_4\left(\frac{1+\sqrt{2}}{2}\right)\right] - 4\left[\mathrm{Li}_4\left(\frac{2-\sqrt{2}}{4}\right) + \mathrm{Li}_4\left(\frac{2+\sqrt{2}}{4}\right)\right],
\end{aligned} \tag{52}$$

where G_4, expressed with the help of the variable r defined in Eq. (41), is given in Eq. (A3).

These results again contain various contributions of polylogarithms with argument $y = -1$, arising from terms of the form $(-1)^n/n^2$ on the r.h.s. of Eq. (51) for J_+ and terms of the form $-\zeta_2/2 - S_2(n-1)$ on the r.h.s. of Eq. (51) for J_-, and with argument $y = r$, arising from the residual terms.

Unfortunately, not all integrals can be computed so straightforwardly. In more complicated cases, the integrations are not separated after expansion to infinite series. We then rely on the PSLQ algorithm [44], which allows one to reconstruct the representation of a numerical result known to very high precision in terms of a linear combination of a set of irrational constants with rational coefficients, if that set is known beforehand. The experience gained with the explicit solution of the simpler integrals helps us to exhaust the relevant sets. In order for the PSLQ algorithm to work in our applications, the numerical values of the integrals must be known up to typically 150 decimal figures. However, for some integrals more accurate determinations are required. The success of the application of the PSLQ algorithm also relies on the fact that only certain combinations of polylogarithms, like G_3 in Eqs. (30) and (42), G_4 in Eq. (A3), and $\tilde{G}_4$ in Eq. (A2) are incorporated as independent structures.

VI. RESULTS

Finally, to get rid of complex polylogarithms, such as $\mathrm{Li}_4[(1+\sqrt{2})/2]$, in the above formulas, we transform all polylogarithms to arguments of value below unity. To this end,

we need transformation formulas through weight four. Some of these formulas are listed in Appendix C. After a laborious calculation, we obtain the final result for the one-loop correction

$$\frac{2}{9}(\pi^2-9)A = \frac{56}{27} + \frac{19}{6}l_2 + \zeta_2\left(-\frac{901}{216} - \frac{2701}{108}l_2 + \frac{253}{24}l_2^2\right) + \frac{11449}{432}\zeta_3 + \frac{59}{576}l_2^4 - \frac{12983}{192}\zeta_4 + \frac{251}{6}\,\mathrm{Li}_4\left(\frac{1}{2}\right) + \tilde{G}_4 + \frac{7}{4}G_4 + \frac{7}{6\sqrt{2}}G_3, \qquad (53)$$

where the constants G_3, G_4, and $\tilde{G}_4$ are specified in Eqs. (42), (A3), and (A2), respectively. Transforming the polylogarithmic functions by means of the formulas given in Appendix C, we arrive at the form of Ref. [29],

$$\begin{aligned}\frac{2}{9}(\pi^2-9)A = {} & \frac{56}{27} + \frac{19}{6}l_2 - \frac{901}{216}\zeta_2 - \frac{2701}{108}\zeta_2 l_2 + \frac{11449}{432}\zeta_3 + \frac{253}{24}\zeta_2 l_2^2 + \frac{913}{64}\zeta_2 l_3^2 + \frac{251}{144}l_2^4 \\ & + \frac{83}{256}l_3^4 - \frac{91}{6}\zeta_3 l_2 - \frac{11303}{192}\zeta_4 \\ & - \frac{21}{4}\zeta_2 l_2 l_r - \frac{49}{16}\zeta_2 l_r^2 + \frac{7}{16}l_2 l_r^3 + \frac{35}{384}l_r^4 - \frac{35}{8}\zeta_3 l_r + \frac{581}{16}\zeta_2\,\mathrm{Li}_2\left(\frac{1}{3}\right) \\ & - \frac{21}{2}l_2\,\mathrm{Li}_3(-r) - \frac{7}{2}l_r\,\mathrm{Li}_3(-r) + \frac{63}{4}l_2\,\mathrm{Li}_3(r) + \frac{63}{8}l_r\,\mathrm{Li}_3(r) \\ & - \frac{249}{32}\,\mathrm{Li}_4\left(-\frac{1}{3}\right) + \frac{249}{16}\,\mathrm{Li}_4\left(\frac{1}{3}\right) + \frac{251}{6}\,\mathrm{Li}_4\left(\frac{1}{2}\right) + 7\,\mathrm{Li}_4(-r) - 7\,\mathrm{S}_{2,2}(-r) \\ & - \frac{63}{4}\,\mathrm{Li}_4(r) + \frac{63}{4}\,\mathrm{S}_{2,2}(r) + \frac{7}{\sqrt{2}}\left[\frac{7}{2}\zeta_2 l_r - \frac{1}{72}l_r^3 - \frac{5}{6}l_r\,\mathrm{Li}_2(r)\right. \\ & \left. + \frac{5}{6}\,\mathrm{Li}_3(r) - \frac{25}{3}\,\mathrm{S}_{1,2}(r) + \frac{2}{3}\,\mathrm{S}_{1,2}(r^2) + \frac{17}{3}\zeta_3\right], \end{aligned} \qquad (54)$$

where r is given in Eq. (41).

From Eqs. (54) and (5), A and C can be numerically evaluated with arbitrary precision,

$$\begin{aligned} A &= -10.286\,614\,808\,628\,262\,240\,150\,169\,210\,991\,253\,179\,644\,007\,490\,228\,232\,410\ldots, \\ C &= 5.517\,027\,491\,729\,858\,271\,378\,866\,098\,665\,005\,181\,944\,001\,421\,860\,702\,103\,921\ldots. \end{aligned} \qquad (55)$$

These numbers agree with the best existing numerical evaluations [16, 17] within the quoted errors.

VII. CONCLUSION

We presented the details of our evaluation of the $\mathcal{O}(\alpha)$ and $\mathcal{O}(\alpha^3\ln\alpha)$ corrections to the total decay width of o-Ps, *i.e.* of the coefficients A and C in Eq. (3), respectively, which

had been presented in our previous Letter [29] in closed analytic form. We discussed the nature and the origin of new irrational constants that appear in the final results. They were shown to be some particular cases of inverse central binomial sums and corresponding generalized polylogarithms. These constants enlarge the class of the known constants in single-scale problems.

The $\mathcal{O}(\alpha^2)$ correction B in Eq. (3) still remains analytically unknown.

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APPENDIX A: DETAILED RESULTS

In this appendix, we present separate results for the integrals I_i of Eq. (25) with $i = 0, \ldots, 7$. Note, that not all of them a finite in the limit $\delta \to 0$. We have:

$$
\begin{aligned}
I_0 &= 204 - 142\zeta_2, \\
I_1 &= 51 + 90l_2 - 228\zeta_2 + \frac{362}{3}\zeta_2 l_2 + \frac{1273}{12}\zeta_3, \\
I_2 &= -40 - \frac{346}{5}\zeta_2 - 72\zeta_2 l_2 + 42\zeta_3 - \frac{17}{\sqrt{2}}G_3, \\
I_3 &= 144\zeta_2 \ln\delta - 59 + 24l_2 + \zeta_2\left(-\frac{219}{2} + 371l_2 - 294l_2^2\right) + 52\zeta_3 - 17l_2^4 - \frac{17121}{16}\zeta_4 \\
&\quad - 408\,\mathrm{Li}_4\left(\frac{1}{2}\right) + 36\tilde{G}_4, \\
I_4 &= -\frac{380}{3} + \zeta_2\left(\frac{328}{15} - 252l_2 + \frac{783}{2}l_2^2\right) + 35\zeta_3 + \frac{279}{16}l_2^4 - \frac{1863}{4}\zeta_4 \\
&\quad + 1026\,\mathrm{Li}_4\left(\frac{1}{2}\right) + 27G_4, \\
I_5 &= -144\zeta_2 \ln\delta - 120 + 6\zeta_2\left(-3 + 6l_2 + 95l_2^2\right) - 357\zeta_3 + \frac{109}{4}l_2^4 - 1398\zeta_4 \\
&\quad + 1464\,\mathrm{Li}_4\left(\frac{1}{2}\right) + 36G_4, \\
I_6 &= 9\ln\delta - \frac{287}{3} + \zeta_2\left(\frac{3781}{6} - 1590l_2 - 288l_2^2\right) + 1328\zeta_3 - 24l_2^4 + \frac{2559}{2}\zeta_4 \\
&\quad - 576\,\mathrm{Li}_4\left(\frac{1}{2}\right) + \frac{35}{\sqrt{2}}G_3, \\
I_7 &= -9\ln\delta + 261 + \zeta_2\left(-\frac{471}{2} + 486l_2\right) - 252\zeta_3 + \frac{315}{16}\zeta_4 + \frac{24}{\sqrt{2}}G_3,
\end{aligned}
\tag{A1}
$$

where G_3 is given in Eqs. (30) and (42), and

$$
\begin{aligned}
\tilde{G}_4 &= \frac{913}{64}\zeta_2 l_3^2 + \frac{581}{16}\zeta_2\,\mathrm{Li}_2\left(\frac{1}{3}\right) + \frac{249}{32}\left[2\,\mathrm{Li}_4\left(\frac{1}{3}\right) - \mathrm{Li}_4\left(-\frac{1}{3}\right)\right] + \frac{83}{256}l_3^4 \\
&\quad - \frac{119}{12}\zeta_3 l_2,
\end{aligned}
\tag{A2}
$$

$$
\begin{aligned}
G_4 &= \frac{15}{16}l_2^4 + \frac{1}{4}l_2 l_r^3 + \frac{5}{96}l_r^4 + 5\zeta_4 + \zeta_2\left(-3l_2 l_r - \frac{7}{4}l_r^2\right) + \zeta_3\left(-3l_2 - \frac{5}{2}l_r\right) \\
&\quad + \left(9l_2 + \frac{9}{2}l_r\right)\mathrm{Li}_3(r) + (-6l_2 - 2l_r)\,\mathrm{Li}_3(-r) - 9\left[\mathrm{Li}_4(r) - \mathrm{S}_{2,2}(r)\right] \\
&\quad + 4\left[\mathrm{Li}_4(-r) - \mathrm{S}_{2,2}(-r)\right].
\end{aligned}
\tag{A3}
$$

From Eqs. (A1) it is clear that $\ln\delta$ cancels in the sum $\sum_{j=0}^{7} I_j$.

APPENDIX B: EXPANSIONS OF Γ AND ψ FUNCTIONS ABOUT HALF-INTEGER ARGUMENTS

In this appendix, we present some useful relations between derivatives of the ψ function with half-integer arguments and the ψ and β functions with integer arguments, and consider the expansion of the Γ function in the vicinity of half-integer arguments.

Starting from the well-known relations between the ψ and β functions,

$$\begin{aligned}\psi(2z) &= \frac{1}{2}\left[\psi\left(z+\frac{1}{2}\right)+\psi(z)\right]+l_2,\\ \beta(2z) &= \frac{1}{2}\left[\psi\left(z+\frac{1}{2}\right)-\psi(z)\right],\end{aligned} \tag{B1}$$

and differentiating them m ($m>0$) times, we have

$$\begin{aligned}2^{m+1}\psi^{(m)}(2z) &= \psi^{(m)}\left(z+\frac{1}{2}\right)+\psi^{(m)}(z),\\ 2^{m+1}\beta^{(m)}(2z) &= \psi^{(m)}\left(z+\frac{1}{2}\right)-\psi^{(m)}(z),\end{aligned} \tag{B2}$$

where $\psi^{(m)}(z)$ denotes the m-th derivative of $\psi(z)$ etc. We can combine Eqs. (B1) and (B2) as

$$\begin{aligned}\psi^{(m)}(z) &= 2^m\left[\psi^{(m)}(2z)-\beta^{(m)}(2z)\right]-\delta_{0m}l_2,\\ \psi^{(m)}\left(z+\frac{1}{2}\right) &= 2^m\left[\psi^{(m)}(2z)+\beta^{(m)}(2z)\right]-\delta_{0m}l_2,\end{aligned} \tag{B3}$$

where δ_{mn} is the Kronecker symbol.

Using the series representations of the ψ and β functions [45],

$$\begin{aligned}\psi(z) &= \psi(1)+(z-1)\sum_{k=0}^{\infty}\frac{1}{(k+1)(k+z)},\\ \beta(z) &= \sum_{k=0}^{\infty}\frac{(-1)^k}{k+z},\end{aligned} \tag{B4}$$

we obtain the following relations:

$$\begin{aligned}\psi(n+1) &= \psi(1)+\mathrm{S}_1(n),\\ \psi^{(m)}(n+1) &= (-1)^m m!\left[\mathrm{S}_{m+1}(n)-\zeta_{m+1}\right],\\ \beta(n+1) &= (-1)^n\left[l_2+\mathrm{S}_{-1}(n)\right],\\ \beta^{(m)}(n+1) &= (-1)^{m+n}m!\left[\mathrm{S}_{-(m+1)}(n)-\mathrm{S}_{-(m+1)}(\infty)\right],\end{aligned} \tag{B5}$$

where $\mathrm{S}_m(n)$ is defined in Eq. (36).

Thus, Eqs. (B3) and (B5) lead to the following results for the "sums" S_m with half-integer arguments [51]:

$$S_1\left(\frac{n}{2}\right) = S_1(n) + (-1)^n S_{-1}(n) - [1-(-1)^n] l_2,$$
$$S_m\left(\frac{n}{2}\right) = 2^{m-1}[S_m(n) + (-1)^n S_{-m}(n)] + [1-(-1)^n](1-2^{m-1})\zeta_m \qquad (m \geq 2). \quad \text{(B6)}$$

These equations are useful for expansions of the Γ function in the vicinities of half-integer arguments. Indeed, using a well-known formula for the expansions of the Γ function about integer values, which was used, *e.g.*, in Ref. [46],

$$\frac{\Gamma(n+1+\delta)}{n!\Gamma(1+\delta)} = \exp\left[-\sum_{k=1}^{\infty}\frac{1}{k}S_k(n)(-\delta)^k\right], \quad \text{(B7)}$$

where γ_E is Euler's constant, we find the corresponding expansions about half-integer values to be

$$\frac{\Gamma(n/2+1+\delta)}{\Gamma(n/2+1)\Gamma(1+\delta)} = \exp\left[-\sum_{k=1}^{\infty}\frac{1}{k}S_k\left(\frac{n}{2}\right)(-\delta)^k\right], \quad \text{(B8)}$$

where $S_m(n/2)$ is given by Eq. (B6). Such expansions are useful in many applications, including those in Ref. [47] and references cited therein.

APPENDIX C: TRANSFORMATIONS OF POLYLOGARITHMS OF WEIGHT FOUR

In this appendix, we present relations between the generalized polylogarithms $\mathrm{S}_{a,b}$ of weight four ($a+b=4$) with different arguments. Transformations at lower weights can be found in the literature [32]. Although the derivation of these formulas is straightforward, we present them here for the convenience of interested readers. At weight four, there are three independent Nielsen polylogarithms, which we choose to be Li_4, $\mathrm{S}_{1,3}$, and $\mathrm{S}_{2,2}$.

1. Relations for the functions with arguments $1-y$ and y:

$$\begin{aligned}
\mathrm{Li}_4(1-y) &= \zeta_4 - \mathrm{S}_{1,3}(y) + \ln(1-y)[\zeta_3 - \mathrm{S}_{1,2}(y)] + \frac{1}{2}\ln^2(1-y)[\zeta_2 - \mathrm{Li}_2(y)] \\
&\quad - \frac{1}{6}\ln^3(1-y)\ln y, \\
\mathrm{S}_{2,2}(1-y) &= \frac{1}{4}\zeta_4 - \mathrm{S}_{2,2}(y) + \ln y\,\mathrm{S}_{1,2}(y) + \ln(1-y)[\zeta_3 - \mathrm{Li}_3(y) + \ln y\,\mathrm{Li}_2(y)] \\
&\quad + \frac{1}{4}\ln^2(1-y)\ln^2 y, \\
\mathrm{S}_{1,3}(1-y) &= \zeta_4 - \mathrm{Li}_4(y) + \ln y\,\mathrm{Li}_3(y) - \frac{1}{2}\ln^2 y\,\mathrm{Li}_2(y) - \frac{1}{6}\ln^3 y\ln(1-y). \qquad \text{(C1)}
\end{aligned}$$

2. Relations for the functions with arguments $-1/y$ and $-y$:

$$\begin{aligned}
\mathrm{Li}_4\left(-\frac{1}{y}\right) &= -\,\mathrm{Li}_4(-y) - \frac{7}{4}\zeta_4 - \frac{1}{2}\zeta_2 \ln^2 y - \frac{1}{24}\ln^4 y,\\
\mathrm{S}_{2,2}\left(-\frac{1}{y}\right) &= \mathrm{S}_{2,2}(-y) - 2\,\mathrm{Li}_4(-y) - \frac{7}{4}\zeta_4 - \ln y[\zeta_3 - \mathrm{Li}_3(-y)] + \frac{1}{24}\ln^4 y,\\
\mathrm{S}_{1,3}\left(-\frac{1}{y}\right) &= -\,\mathrm{S}_{1,3}(-y) + \mathrm{S}_{2,2}(-y) - \mathrm{Li}_4(-y) - \zeta_4 - \ln y[\mathrm{S}_{1,2}(-y) - \mathrm{Li}_3(-y)]\\
&\quad - \frac{1}{2}\ln^2 y\,\mathrm{Li}_2(-y) - \frac{1}{24}\ln^4 y. \qquad \text{(C2)}
\end{aligned}$$

3. Relations for the functions with arguments $(y-1)/y$ and y:

$$\begin{aligned}
\mathrm{Li}_4\left(\frac{y-1}{y}\right) &= \mathrm{Li}_4(y) + \mathrm{S}_{1,3}(y) - \mathrm{S}_{2,2}(y) - \frac{7}{4}\zeta_4 + \ln(1-y)[\mathrm{S}_{1,2}(y) - \mathrm{Li}_3(y)]\\
&\quad + \frac{1}{2}\ln^2(1-y)\,\mathrm{Li}_2(y) - \frac{1}{2}\zeta_2 \ln^2\frac{1-y}{y} + \frac{1}{24}\ln^4(1-y)\\
&\quad - \frac{1}{24}\ln^4\frac{1-y}{y},\\
\mathrm{S}_{2,2}\left(\frac{y-1}{y}\right) &= 2\,\mathrm{Li}_4(y) - \mathrm{S}_{2,2}(y) - \frac{7}{4}\zeta_4 + \ln y\,\mathrm{S}_{1,2}(y) + \ln\frac{1-y}{y}\zeta_3 - \ln[(1-y)y]\,\mathrm{Li}_3(y)\\
&\quad + \ln y \ln(1-y)\,\mathrm{Li}_2(y) + \frac{1}{4}\ln^2 y \ln^2(1-y) - \frac{1}{6}\ln^3 y \ln(1-y)\\
&\quad + \frac{1}{24}\ln^4 y,\\
\mathrm{S}_{1,3}\left(\frac{y-1}{y}\right) &= \mathrm{Li}_4(y) - \zeta_4 - \ln y\,\mathrm{Li}_3(y) + \frac{1}{2}\ln^2 y\,\mathrm{Li}_2(y) + \frac{1}{6}\ln^3 y \ln(1-y)\\
&\quad - \frac{1}{24}\ln^4 y. \qquad \text{(C3)}
\end{aligned}$$

4. Relations for the functions with arguments $y/(y-1)$ and y:

$$\begin{aligned}
\mathrm{Li}_4\left(\frac{y}{y-1}\right) &= \mathrm{S}_{2,2}(y) - \mathrm{Li}_4(y) - \mathrm{S}_{1,3}(y) + \ln(1-y)[\mathrm{Li}_3(y) - \mathrm{S}_{1,2}(y)]\\
&\quad - \frac{1}{2}\ln^2(1-y)\,\mathrm{Li}_2(y) - \frac{1}{24}\ln^4(1-y),\\
\mathrm{S}_{2,2}\left(\frac{y}{y-1}\right) &= \mathrm{S}_{2,2}(-y) - 2\,\mathrm{S}_{1,3}(y) - \ln(1-y)\,\mathrm{S}_{1,2}(y) + \frac{1}{24}\ln^4(1-y),\\
\mathrm{S}_{1,3}\left(\frac{y}{y-1}\right) &= -\,\mathrm{S}_{1,3}(y) - \frac{1}{24}\ln^4(1-y). \qquad \text{(C4)}
\end{aligned}$$

5. Relations for the functions with arguments $1/(1+y)$ and $-y$:

$$\begin{aligned}
\mathrm{Li}_4\left(\frac{1}{1+y}\right) &= \mathrm{S}_{1,3}(-y) + \zeta_4 + \ln(1+y)[\mathrm{S}_{1,2}(-y) - \zeta_3] + \frac{1}{2}\ln^2(1+y)[\mathrm{Li}_2(-y) + \zeta_2] \\
&\quad + \frac{1}{6}\ln^3(1+y)\ln y - \frac{1}{24}\ln^4(1+y), \\
\mathrm{S}_{2,2}\left(\frac{1}{1+y}\right) &= 2\,\mathrm{S}_{1,3}(-y) - \mathrm{S}_{2,2}(-y) + \frac{1}{4}\zeta_4 + + \ln[y(1+y)]\,\mathrm{S}_{1,2}(-y) \\
&\quad - \ln(1+y)[\mathrm{Li}_3(-y) + \zeta_3] + \ln(1+y)\ln y\,\mathrm{Li}_2(-y) + \frac{1}{4}\ln^2(1+y)\ln^2 y \\
&\quad - \frac{1}{6}\ln^3(1+y)\ln y + \frac{1}{24}\ln^4(1+y), \\
\mathrm{S}_{1,3}\left(\frac{1}{1+y}\right) &= \mathrm{S}_{1,3}(-y) - \mathrm{S}_{2,2}(-y) + \mathrm{Li}_4(-y) + \zeta_4 + \ln y[\mathrm{S}_{1,2}(-y) - \mathrm{Li}_3(-y)] \\
&\quad + \frac{1}{2}\ln^2 y\,\mathrm{Li}_2(-y) + \frac{1}{24}\ln^4 y - \frac{1}{24}\ln^4\frac{1+y}{y}. \qquad \text{(C5)}
\end{aligned}$$

Equations (C1) and (C2) were directly obtained from Ref. [32], where they are presented for the generalized polylogarithms $\mathrm{S}_{a,b}$ with arbitrary values of a and b, but in some complicated form less convenient for applications. Equations (C3)–(C5) were found by iterated application of Eqs. (C1) and (C2) and equations from Ref. [32]. They are simple and useful for applications together with equations for $\mathrm{S}_{a,b}$ from Ref. [32], with the constraints $a+b=2$ or $a+b=3$.

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[48] Equation (18) corrects a misprint in Eq. (15) of Ref. [29], which is, however, inconsequential because the difference between these expressions cancels due to the $x_1 \leftrightarrow x_3$ symmetry.

[49] The subscript of the universal contribution G_3 is to indicate that all its parts carry weight three.

[50] Some examples were already considered in Ref. [37].

[51] We may use Eq. (B5) as definition of the "sums" S_m with half-integer arguments.