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The photon-energy spectrum in $B \rightarrow X_s \gamma$ to $N^3\text{LO}$: light-fermion and large- N_c corrections

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ABSTRACT: We consider the photon-energy spectrum of the inclusive radiative decay $B \rightarrow X_s \gamma$, induced by the electromagnetic dipole operator O_7 , to next-to-next-to-next-to-leading order and calculate the complete corrections for light fermions, for the contributions with two closed massive fermion loops, and for the limit of large QCD colour factors N_c in the remaining part. We discuss the integrated decay rate both without and with a cut on the photon energy. In addition to the on-shell renormalization of the bottom-quark mass, we also consider the kinetic mass and the MSR mass schemes. The latter two lead to an improved perturbative behaviour of the decay rate.

KEYWORDS: Bottom Quarks, Higher-Order Perturbative Calculations, Rare Decays, Effective Field Theories

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1 Introduction

The inclusive radiative decay $B \rightarrow X_s \gamma$ is a cornerstone of flavour physics, providing a high-precision test of the Standard Model (SM) and a powerful probe of potential new-physics effects.

At the quark level, this process is mediated by the flavour-changing neutral-current (FCNC) transition $b \rightarrow s \gamma$, which is a loop-suppressed process subject to Glashow-Iliopoulos-Maiani (GIM) mechanism, although the suppression is partially lifted by the large top-quark mass.

From a theoretical point of view, the inclusive nature of the $B \rightarrow X_s \gamma$ decay allows the dominant contribution to be analysed systematically using the heavy-quark expansion combined with perturbative quantum chromodynamics (QCD), leading to precise SM predictions. For the $O_7 - O_7$ contribution, the leading local nonperturbative corrections arise at order $\Lambda_{\text{QCD}}^2/m_b^2$ [1]. The complete decay rate, however, also receives nonlocal resolved-photon contributions involving other operators in the effective Hamiltonian [2–4], as well as contributions from collinear photon emission off energetic light partons [5, 6]. These effects are not fully captured by the local operator product expansion and constitute an important source of residual hadronic uncertainty.

Furthermore, unlike $b \rightarrow s \ell^+ \ell^-$ transitions, the photon-energy spectrum in $B \rightarrow X_s \gamma$ does not exhibit strong resonant structures associated with intermediate charmonium states. Photons from cascade decays, e.g. $B \rightarrow X_s J/\psi$ followed by $J/\psi \rightarrow X \gamma$, nevertheless contribute to the measured photon-energy spectrum but are controlled by imposing a sufficiently high lower-cut on E_γ , preserving $B \rightarrow X_s \gamma$ as one of the theoretically cleanest FCNC observables.

On the experimental side, the branching fraction of $B \rightarrow X_s \gamma$ has been measured with steadily improving accuracy [7–13] and is in good agreement with SM predictions [14–16].

The Belle II experiment is expected to reach a precision of roughly 2.5% on the branching fraction [17]. To match this level of experimental accuracy and to fully exploit the sensitivity of this observable to new physics, further improvements in the theoretical description of $B \rightarrow X_s \gamma$ are clearly required.

In this work, we concentrate on the photon-energy spectrum in $B \rightarrow X_s \gamma$.

Since experimental analyses impose a lower cut on the photon energy of about 1.8–2.0 GeV in the B -meson rest frame, an accurate theoretical prediction for the differential decay rate, including perturbative QCD corrections, is essential for a meaningful comparison with data.

Within soft-collinear effective theory (SCET), the photon spectrum in the endpoint region is governed by the leading shape function [18–20], a universal nonperturbative object that encapsulates the QCD dynamics close to the kinematic boundary and plays a role similar to that of parton distribution functions. The same shape function also appears in the theoretical description of inclusive semileptonic decays $B \rightarrow X_u \ell \bar{\nu}_\ell$ and is thus a crucial ingredient in determinations of $|V_{ub}|$. A robust extraction of the shape function from experimental data hinges on an accurate control of the short-distance contributions to the spectrum, including higher-order perturbative effects.

The SIMBA collaboration has performed a fit to the $B \rightarrow X_s \gamma$ photon spectrum using fixed-order theoretical predictions at next-to-next-to-leading order (NNLO), next-to-next-to-leading-logarithmic (NNLL) resummation plus all singular terms at $O(\alpha_s^2)$ (NNLL') [21, 22]. More recently, this framework was extended to next-to-next-to-next-to-leading logarithmic (N³LL') accuracy in ref. [23]. However, that analysis did not yet include the three-loop hard function, corresponding to the $b \rightarrow s \gamma$ form factor, nor the complete fixed-order N³LO result for the photon spectrum. These missing ingredients were therefore treated as nuisance parameters, and their variation induced an additional theory uncertainty. The hard function at $O(\alpha_s^3)$ has since been computed in ref. [24].

At the parton level, the photon-energy spectrum in $B \rightarrow X_s \gamma$ is known up to NNLO for the contributions arising from the interference of the electromagnetic and chromomagnetic dipole operators [25–27]. For the integrated rate, the interference between four-quark current-current operators and the electromagnetic dipole operator, only an interpolation between the heavy-charm limit [28, 29] and the massless-charm limit [15] is currently available. Partial NNLO results for the two-body contribution with exact charm-mass dependence have been reported recently [30–33]. In addition, perturbative corrections to the matching [34] and renormalization-group evolution [35–37] of the operators in the $\Delta B = \Delta S = 1$ effective Hamiltonian are known through NNLO.

In this paper, we take a first step towards a full N³LO determination of the photon-energy spectrum in QCD. We compute the partonic contribution of the electromagnetic dipole operator O_7 to $d\Gamma/dE_\gamma$ through $O(\alpha_s^3)$ and present analytic expressions for the fermionic colour structures proportional to n_1^2 , n_1 , and n_1^2 , as well as for the leading-colour bosonic contribution proportional to N_c^3 at N³LO. In particular, we evaluate both the singular and non-singular terms in the spectrum arising from real-emission corrections. By combining these results with the virtual contributions inferred from the three-loop tensor form factors of ref. [24], we also obtain the O_7 contribution to the integrated decay rate through $O(\alpha_s^3)$.

The paper is organized as follows: In the next section we introduce the relevant parts of the effective theory necessary to obtain the photon-energy spectrum and explain the strategy for the evaluation of virtual and real corrections. The latter is the main new result obtained in this paper. In section 3 we describe in detail the techniques, which we use to extract the singular and regular part of the spectrum. Our analytical and numerical results are presented in section 4 and the conclusions can be found in section 5. In the appendix we provide useful formulae in connection to the plus distributions and explicit analytic results for the regular part of the photon spectrum.

2 Photon-energy spectrum to higher orders in QCD

We consider the decay of a B meson into a photon and any hadronic final state containing a strange quark: $B \rightarrow X_s \gamma$. To leading order in the heavy quark expansion (HQE) the decay is described by the decay $b \rightarrow X_s \gamma$ of a free bottom quark. In the SM the decay is governed by the $\Delta B = \Delta S = 1$ effective Lagrangian

$$\mathcal{L}_{\text{eff}} = \frac{4G_F}{\sqrt{2}} V_{tb} V_{ts}^* \left[\sum_{i=1}^6 C_i(\mu) O_i + C_7(\mu) O_7 + C_8(\mu) O_8 \right], \quad (2.1)$$

where $O_1, \dots, O_6$ are the usual current-current and QCD penguin operators, while O_7 and O_8 are the electro- and chromo-magnetic dipole operators. In this paper, we consider the contribution to the partonic $b \rightarrow X_s \gamma$ decay rate originating only from the electromagnetic dipole operator

$$O_7 = \frac{e}{16\pi^2} \bar{m}_b \left(\bar{s} \sigma^{\mu\nu} P_R b \right) F_{\mu\nu}. \quad (2.2)$$

Here $F_{\mu\nu}$ is the electromagnetic field strength tensor, e is the electromagnetic coupling constant with $\alpha_{\text{em}} = e^2/(4\pi)$, $\sigma_{\mu\nu} = i[\gamma_\mu, \gamma_\nu]/2$, and the bottom quark mass $\bar{m}_b \equiv \bar{m}_b(\mu)$ in the $\overline{\text{MS}}$ scheme.

The partonic photon energy spectrum can be written in terms of the normalized photon energy $x = 2E_\gamma/m_b$ in the b rest frame as

$$\frac{d\Gamma}{dx} = \frac{G_F^2 \alpha_{\text{em}} \bar{m}_b(\mu) m_b^3}{32\pi^4} |V_{tb} V_{ts}^*|^2 \sum_{i,j} C_i(\mu) C_j(\mu) \frac{dG_{ij}(x, \mu)}{dx}, \quad (2.3)$$

where $C_i(\mu)$ are the Wilson coefficients in the effective theory evaluated at the scale $\mu \simeq m_b$. We will focus on the function dG_{77}/dx and compute it up to N³LO. In the following, we will denote the contribution of this term to the decay rate as $d\Gamma_{77}/dx$. As a by-product, we will also obtain the prediction for the integrated rate by integrating eq. (2.3) over the phase space. To higher orders in QCD, the spectrum $d\Gamma_{77}/dx$ receives contributions from the two-body decay $b \rightarrow s\gamma$, which we will simply refer to as “virtual corrections”, as well as from multi-parton emissions $b \rightarrow s\gamma g$, $b \rightarrow s\gamma gg$, etc. which we denote as “real corrections.”

Virtual corrections. For the evaluation of the virtual corrections to the spectrum, we make use of the results for the QCD heavy-to-light form factors up to $O(\alpha_s^3)$ presented in ref. [24]. In particular, we concentrate on the tensor current

$$j_t^{\mu\nu} = i\bar{\psi}_Q \sigma^{\mu\nu} \psi_q. \quad (2.4)$$

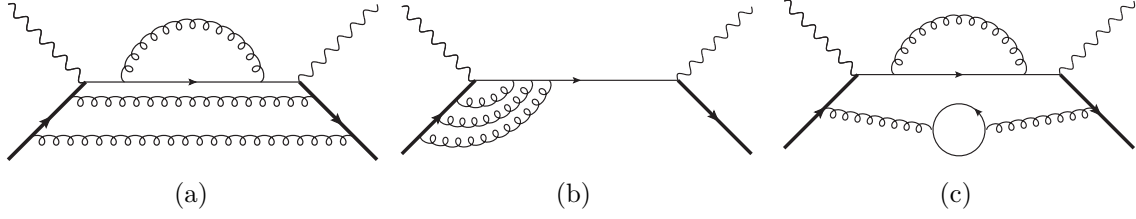


Figure 1. Sample Feynman diagrams contributing to the forward scattering amplitude of $b\gamma \rightarrow b\gamma$. Thin (bold) lines denote the strange (bottom) quarks. Their imaginary parts provide the real emission contribution to the photon energy spectrum in $b \rightarrow X_s \gamma$ at partonic level. Their full discontinuity, which also involves cuts through single reducible s -quark propagators (see e.g. (b)), reproduces the virtual contributions as well. We choose to include the latter via the heavy-to-light form factor, as described in the text.

Here we follow the notation of ref. [24] and define the form factors as

$$\begin{aligned} \Gamma_{\mu\nu}^t(q_1, q_2) = & iF_1^t(q^2)\sigma_{\mu\nu} + \frac{F_2^t(q^2)}{m}(q_{1,\mu}\gamma_\nu - q_{1,\nu}\gamma_\mu) + \frac{F_3^t(q^2)}{m}(q_{2,\mu}\gamma_\nu - q_{2,\nu}\gamma_\mu) \\ & + \frac{F_4^t(q^2)}{m^2}(q_{1,\mu}q_{2,\nu} - q_{1,\nu}q_{2,\mu}). \end{aligned} \quad (2.5)$$

The momentum q_1 is the incoming momentum of the massless quark and q_2 is the outgoing momentum of the heavy quark. Furthermore, we have $q = q_1 - q_2$, with $q^2 = q_1^2 = 0$ and $q_2^2 = m^2$.

The virtual corrections to the differential rate can be obtained from the form factors calculated at $q^2 = 0$. We obtain the tree-level decay rate for $b \rightarrow s\gamma$ using as Feynman rule $-2iP_R\Gamma_{\mu\nu}^t p_\gamma^\mu$, where we identify $q_1 = -p_s$, $q_2 = -p_b$, and $q = p_\gamma$. The expression for the virtual corrections in terms of the tensor form factor is given by

$$\frac{dG_{77}^{\text{virt}}}{dx} = \frac{1-\epsilon}{4} \frac{\Gamma(1-\epsilon)e^{\epsilon\gamma_E}}{\Gamma(2-2\epsilon)} \left[2F_1^t(0) - F_2^t(0) - F_3^t(0) \right]^2 \delta(1-x). \quad (2.6)$$

Real corrections. To compute the real-emission contributions with the emission of n additional partons, we consider forward scattering amplitudes for the process $b\gamma \rightarrow b\gamma$ and extract their imaginary part (see the sample diagrams in figure 1).

The differential decay rate of $b \rightarrow X_s \gamma$ can be written as

$$d\Gamma = \frac{(2\pi)^d}{2m_b} \overline{|\mathcal{M}|^2} d\Phi_{n+2}(p_b; p_\gamma, p_s, p_1, \dots, p_n), \quad (2.7)$$

where p_γ and p_s denote the four-momenta of the photon and strange quark in the rest frame of the b quark, respectively, and $d = 4 - 2\epsilon$ is the space-time dimension. The momenta of the additional real partons in the hadronic final state X_s are denoted by $p_1, \dots, p_n$. The quantity $\overline{|\mathcal{M}|^2}$ represents the squared matrix element, averaged over the spins of the initial state and summed over those of the final state.

A generic n -body phase space is defined as

$$d\Phi_n(P; p_1, \dots, p_n) = \delta^{(d)}\left(P - \sum_{i=1}^n p_i\right) \prod_{i=1}^n \frac{d^{d-1}p_i}{(2\pi)^{d-1}2E_i}. \quad (2.8)$$

At leading order, the decay $b \rightarrow X_s \gamma$ is described by the two-body phase space $d\Phi_2$. At higher orders in QCD, where n additional partons are emitted, the $(n+2)$ -particle phase space can be written as

$$\begin{aligned} d\Phi_{n+2} &= \frac{d^{d-1}p_\gamma}{(2\pi)^{d-1}2E_\gamma} \frac{d^{d-1}p_s}{(2\pi)^{d-1}2E_s} \prod_{i=1}^n \frac{d^{d-1}p_i}{(2\pi)^{d-1}2E_i} \delta^{(d)} \left(p_b - p_\gamma - p_s - \sum_{i=1}^n p_i \right) \\ &= \frac{E_\gamma^{d-3} dE_\gamma d\Omega_{d-1}}{2(2\pi)^{d-1}} \frac{d^{d-1}p_s}{(2\pi)^{d-1}2E_s} \prod_{i=1}^n \frac{d^{d-1}p_i}{(2\pi)^{d-1}2E_i} \delta^{(d)} \left(p_b - p_\gamma - p_s - \sum_{i=1}^n p_i \right). \end{aligned} \quad (2.9)$$

After integrating over the d -dimensional solid angle of the photon momentum,

$$\int d\Omega_{d-1} = (4\pi)^{1-\epsilon} \frac{\Gamma(1-\epsilon)}{\Gamma(2-2\epsilon)}, \quad (2.10)$$

the differential decay rate with respect to the photon energy E_γ can be cast into the form

$$\begin{aligned} \frac{1}{E_\gamma^{1-2\epsilon}} \frac{d\Gamma}{dE_\gamma} &= \frac{1}{8m\pi^{2-\epsilon}} \frac{\Gamma(1-\epsilon)}{\Gamma(2-2\epsilon)} \\ &\times (2\pi)^d \int |\mathcal{M}|^2 \frac{d^{d-1}p_s}{2E_s(2\pi)^{d-1}} \prod_{i=1}^n \frac{d^{d-1}p_i}{(2\pi)^{d-1}2E_i} \delta^d \left(p_b - p_\gamma - p_s - \sum_{i=1}^n p_i \right). \end{aligned} \quad (2.11)$$

In order to make use of modern techniques for multi-loop calculations, it is advantageous to convert the integration over the phase space in eq. (2.11) into a loop integration. In ref. [25], this has been achieved by the technique of reverse unitarity [38], effectively converting the constraint on the photon momentum $\delta(p_b \cdot p_\gamma - m_b E_\gamma)$ to a propagator and taking the imaginary part of the integrals. We proceed in a different way. If we perform the replacement $p_\gamma \rightarrow p'_\gamma = -p_\gamma$, thereby interpreting the outgoing photon as an incoming one, the right-hand side of eq. (2.11) — namely the factor isolated on the second line — can be identified with the total cross section for the scattering process $b(p_b) + \gamma(p'_\gamma) \rightarrow X_s(p_b + p'_\gamma)$ with $(p_b + p'_\gamma)^2 > m_b^2$ and at fixed centre-of-mass energy defined by $p_b \cdot p'_\gamma = m_b E'_\gamma = m_b^2 x'/2$. This total cross section can be computed using the optical theorem, by evaluating the imaginary part of the forward scattering amplitude for $b(p_b) + \gamma(p'_\gamma) \rightarrow b(p_b) + \gamma(p'_\gamma)$. Afterwards, we identify $x' = -x = -2E_\gamma/m_b$ to recover the decay kinematics.

3 Technical details

Generation of the amplitude. We generate the forward scattering diagrams with **qgraf** [39] and generate **FORM** [40, 41] code for the calculation of the amplitude with **tapir** [42] and **exp** [43, 44]. **tapir** also generates partial fraction identities for the denominators, which are necessary due to the forward scattering kinematics. The Dirac and colour algebra [45] is performed with **FORM**. Due to the partial fraction decomposition we end up with a large number of integral families which are not all independent. We use **feynson** [46] to map them to a minimal set. In total we find 1, 6, and 44 integral families at one-, two- and three-loop order, respectively.

IBP reduction. At one- and two-loop order, we perform a full integration-by-parts (IBP) reduction [47–49] of the scalar integrals with *Kira* [50–52]. We find 3 and 42 master integrals, respectively. At two-loop order, 18 out of the 42 master integrals do not have an imaginary part and can therefore be discarded.

At three loops, the approach of first performing the full reduction to master integrals and discarding master integrals without imaginary part at a later stage leads to prohibitively expensive IBP reductions. Therefore, we refine our approach in the following way. Before reduction, we determine every sector of a family which does not generate an imaginary part and supply this sector as vanishing sector to *Kira*. This way, integrals without imaginary part are dropped in every step, significantly reducing the complexity of the reduction (see also ref. [53]). Furthermore, the number of master integrals reduces drastically. The use of *Kira* 3 [52, 54] with *FireFly* [55, 56] as backend for finite field techniques [57–59] was essential for performing the IBP reductions at three-loop order. In order to facilitate the efficient reduction of the master integrals, we also search for a basis of master integrals, in which the denominators factorize in d and x [60, 61]. To find suitable candidates for this search, we perform simpler test reductions with *Kira* and use *ImproveMasters.m* [60]¹ to find a suitable basis. In total we find 987 master integrals for the full amplitude. Restricting ourselves to the large- N_c limit, only 132 master integrals are needed. For the fermionic pieces with at least one massless fermion loop, we need 82 master integrals, and for the n_h^2 piece only 2 master integrals contribute. Eliminating the overlap between these three contributions results in 158 master integrals which have to be computed.

Calculation of the master integrals. To compute the master integrals, we derive differential equations in x [63–66]. We employ *LiteRed* [67, 68] to differentiate the master integrals with respect to x and use reduction tables obtained by *Kira* to establish the differential equations.

The calculation of the master integrals is complicated by the soft singularity in the limit $y = 1 - x \rightarrow 0$. In this limit the master integrals behave as

$$\vec{I}(\epsilon, y) = \sum_n y^{m+n\epsilon} \vec{J}(\epsilon, y), \quad (3.1)$$

which leads to distributions via the identities given in appendix A. Therefore, we cannot simply calculate the master integrals as functions of y , but need to separate them into the different branches of the asymptotic expansion around $y \rightarrow 0$. In general, we find branches with $n = 1, 2, \dots, 2l$, where l is the loop order under consideration. Note that we do not have to consider the region with $n = 0$, since this region does not contribute to the imaginary part of the integral.

To solve the integrals, we do the following:

- We solve the integrals without separation into the different branches. To do this we use the algorithm outlined in ref. [69] to solve the coupled system of first order differential equations in the variable $y = 1 - x$, i.e. we do not search for a canonical form of the differential equation, but solve the differential equations by decoupling to higher-order

¹It was shipped together with *FIRE* from version 6.4.1 until version 6.6 [62].

differential operators and factorization. This provides us with an analytic solution in terms of iterated integrals. At one- and two-loop order it is quite straightforward to obtain boundary conditions for $y \rightarrow 0$ via the method of regions [70], direct integration, and Mellin-Barnes methods, see e.g. refs. [71, 72].

At three-loop order we proceed in a slightly different way. We use `AMFlow` [73–76] to obtain initial conditions at the point $y = 2/11$ with 100 digits of precision. We compare these results with the numerical evaluation of the formal solutions of the master integrals in terms of iterated integrals, which still depend on undetermined boundary coefficients. For the numerical evaluation of the iterated integrals at $y = 2/11$, we can perform a deep series expansion up to $\mathcal{O}(y^{200})$. We observe that this is sufficient to obtain 100 significant digits, and we can directly compare to the numerical evaluations with `AMFlow`. We found this approach to be more convenient, since for $y > 0$ functions beyond multiple polylogarithms contribute to the results of the master integrals. In the end, we are able to obtain analytic boundary conditions using the PSLQ algorithm [77], and we find that only (multiple) ζ values appear.

- In a second step, we insert for each branch of the asymptotic expansion an ansatz of the form in eq. (3.1), where $\vec{J}(\epsilon, y)$ has a Taylor expansion around $y = 0$, into the differential equation and express the result of each branch in terms of a minimal number of boundary conditions. We choose as starting power $m = -6$ such that J has indeed a Taylor and not a Laurent expansion. By demanding that the sum of all branches recovers the expansion of the full master integrals we calculated in the step before, we can determine the majority of boundary conditions of the different branches. For some master integrals we are not able to fix all boundary conditions in this way. In these cases we either calculate the boundary conditions directly with the help of the method of regions, use consistency conditions at $y \rightarrow 1$, or expand the master integrals to higher orders in ϵ .
- Having at our disposal the analytic expansion of each master integral around $y = 0$ separated into branches, we solve the full differential equations again by using as boundary conditions these results for each branch individually. In this way we can express all master integrals as sums over all branches.

At one- and two-loop order we see that multiple polylogarithms of argument $y = 1 - x$ are enough to solve the differential equations. The letters are given by:

$$f_0(t) = \frac{1}{t}, \quad f_{-1}(t) = \frac{1}{1+t}, \quad f_1(t) = \frac{1}{1-t}, \quad f_2(t) = \frac{1}{2-t}. \quad (3.2)$$

At the three-loop level we find additionally

$$f_a(t) = \sqrt{4-t}\sqrt{t}, \quad f_b(t) = \frac{\sqrt{4-t}\sqrt{t}}{1-t}. \quad (3.3)$$

We use the definition of the iterated integrals

$$H_{w_1, \vec{w}}(x) = \int_0^x dt f_{w_1}(t) H_{\vec{w}}(t), \quad (3.4)$$

with the usual regularizations for the letter $f_0(t)$, i.e.

$$H_{\underbrace{0, \dots, 0}_{n \text{ times}}}(x) = \frac{1}{n!} \log^n(x). \quad (3.5)$$

It is interesting to note that the master integrals for the leading- N_c term do depend on the new letters, the final amplitude, however, is free of them. The full complexity is only reached for the colour factors linear in n_l . The colour factors which are not covered here also depend on more complicated geometries, like elliptic functions and beyond.

Note that it is in principle possible to rationalize the letters containing square-roots by a variable change of the argument, e.g. by changing to the variable $\omega = -(1-y)^2/y$. This change of variables enables the numerical evaluation with established tools like `ginac` [78, 79], but introduces many more letters and leads to a much bigger expression of the amplitude. For an efficient numerical evaluation, we therefore expand the amplitude around $x = 0$ and $x = 1$ to 100 terms in each limit. Both expansions have a radius of convergence of radius 1 and agree to 30 digits at the intermediate point $x = 1/2$. The expansion around $x = 0$ requires an analytic continuation, which we carry out with `HarmonicSums` [80–91] and `Sigma` [92, 93]. Here, we encounter the constant

$$c_1 = H_a(1)H_{a,2,1}(1) - H_{a,a,2,1}(1) = 0.2598851170\dots \quad (3.6)$$

For the total decay rate in section 4.2 we also encounter the constants

$$\begin{aligned} c_2 &= H_a(1)H_{a,2,0}(1) - H_{a,a,2,0}(1) = -0.4018313022\dots \\ c_3 &= H_a(1)H_{a,2,1,0}(1) - H_{a,a,2,1,0}(1) = -0.3288306064\dots \end{aligned} \quad (3.7)$$

In the supplementary files we provide numerical evaluations of these constants with 1000 significant digits. Expressing these constants in terms of Goncharov polylogarithms does not lead to a more compact notation. However, if the letter $f_2(t)$ is absent, the rationalization leads only to harmonic and cyclotomic harmonic polylogarithms [84, 94] for which the transcendental constants at unit argument are known [84, 95]. We have checked, using the `PSLQ` algorithm, that the constants in eqs. (3.6) and (3.7) are linearly independent to these ones.

Singular and regular parts of the amplitude. In order to separate the singular and regular parts in the amplitude we proceed as follows. In a first step, we insert the master integrals separated into the different branches as described in the previous section into the amplitude. Next, we expand the amplitude for $y \rightarrow 0$ and collect all contributions that behave as $1/y^{(k-n\epsilon)}$ with $k > 0$. In our case, we have $k \leq 3$ and $1 \leq n \leq 6$. These contributions define the singular part of the amplitude, which we denote by

$$\left. \frac{1}{E_\gamma} \frac{dG_{77}}{dE_\gamma} \right|_{\text{sing}}. \quad (3.8)$$

The regular part is then obtained via

$$\left. \frac{1}{E_\gamma} \frac{dG_{77}}{dE_\gamma} \right|_{\text{reg}} = \frac{1}{E_\gamma} \frac{dG_{77}}{dE_\gamma} - \left. \frac{1}{E_\gamma} \frac{dG_{77}}{dE_\gamma} \right|_{\text{sing}}, \quad (3.9)$$

which has by construction a regular behaviour for $y \rightarrow 0$. Furthermore, it is finite for $\epsilon \rightarrow 0$ after renormalization.

At this point we use the relations from appendix A to rewrite the singular part in terms of distributions. Afterwards, the coefficients of the plus distributions are finite and the limit $\epsilon \rightarrow 0$ can be taken. The coefficients of $\delta(y)$ still contain poles in ϵ up to $1/\epsilon^6$. They cancel against the virtual corrections discussed in the previous section.

4 Results

4.1 Analytic expressions for the spectrum

In the following we present the analytic results of our calculation for $\mu = m_b$. The differential decay rate can be written as

$$\frac{d\Gamma_{77}}{dx} = \Gamma_0 m_b^3 \bar{m}_b^2(m_b) |C_7(m_b)|^2 \left[\delta(1-x) + \frac{\alpha_s}{\pi} Y_1(x) + \left(\frac{\alpha_s}{\pi}\right)^2 Y_2(x) + \left(\frac{\alpha_s}{\pi}\right)^3 Y_3(x) \right], \quad (4.1)$$

with $\Gamma_0 = \alpha_{\text{em}} G_F^2 |V_{tb} V_{ts}^*|^2 / 32\pi^4$ where the expansion coefficients have the form

$$Y_i(x) = Y_i^\delta \delta(1-x) + Y_i^+(x) + Y_i^{\text{reg}}(x). \quad (4.2)$$

The first two terms correspond to distributions, while the last term is the regular part of the spectrum. At NLO, NNLO, and N³LO the terms proportional to the δ -distribution are given by

$$Y_1^\delta = -C_F \left(\frac{5}{4} + \frac{\pi^2}{3} \right), \quad (4.3)$$

$$\begin{aligned} Y_2^\delta = & C_A C_F \left(\frac{55\zeta_3}{48} + \frac{143\pi^4}{2880} - \frac{215\pi^2}{864} - \frac{11987}{1728} - \frac{37}{24}\pi^2 \ln(2) \right) \\ & + C_F^2 \left(-\frac{33\zeta_3}{8} + \frac{59\pi^4}{1440} - \frac{167\pi^2}{96} + \frac{989}{192} + \frac{37}{12}\pi^2 \ln(2) \right) \\ & + C_F T_F n_h \left(-\frac{\zeta_3}{3} - \frac{29\pi^2}{54} + \frac{3563}{648} \right) + C_F T_F n_l \left(\frac{\zeta_3}{3} + \frac{91\pi^2}{216} + \frac{631}{432} \right), \end{aligned} \quad (4.4)$$

$$\begin{aligned} Y_3^\delta = & C_A C_F T_F n_l \left(-\frac{1}{72}\pi^2 \zeta_3 + \frac{221\zeta_3}{432} - \frac{43\zeta_5}{12} - \frac{67\text{Li}_4\left(\frac{1}{2}\right)}{9} + \frac{19\pi^4}{648} + \frac{4001\pi^2}{1944} + \frac{320753}{23328} \right. \\ & - \frac{67\log^4(2)}{216} - \frac{23}{54}\pi^2 \ln^2(2) + \frac{59}{18}\pi^2 \ln(2) \Big) + C_F T_F^2 n_h n_l \left(\frac{4\zeta_3}{27} - \frac{\pi^4}{405} + \frac{443\pi^2}{972} \right. \\ & - \frac{13243}{2916} \Big) + C_F T_F^2 n_h^2 \left(\frac{26\zeta_3}{9} - \frac{\pi^4}{270} + \frac{2\pi^2}{15} - \frac{374}{81} \right) + C_F T_F^2 n_l^2 \left(-\frac{32\zeta_3}{27} - \frac{\pi^4}{108} \right. \\ & - \frac{1061\pi^2}{1944} - \frac{12727}{11664} \Big) + C_F^2 T_F n_l \left(\frac{5\pi^2 \zeta_3}{18} + \frac{1073\zeta_3}{72} + \frac{10\zeta_5}{3} + \frac{134\text{Li}_4\left(\frac{1}{2}\right)}{9} - \frac{6047\pi^4}{12960} \right. \\ & + \frac{1181\pi^2}{324} - \frac{13141}{2592} + \frac{67\ln^4(2)}{108} + \frac{23}{27}\pi^2 \ln^2(2) - \frac{59}{9}\pi^2 \ln(2) \Big) + N_c^3 \left(-\frac{19\zeta_3^2}{64} \right. \\ & + \frac{41\pi^2 \zeta_3}{192} - \frac{16391\zeta_3}{3456} + \frac{113\zeta_5}{48} - \frac{2455\pi^6}{290304} + \frac{111289\pi^4}{414720} - \frac{277753\pi^2}{124416} - \frac{11206753}{1492992} \Big) \\ & + \mathcal{O}(N_c^2, n_h). \end{aligned} \quad (4.5)$$

The plus distributions read

$$Y_1^+(x) = -C_F \left(\frac{7\mathcal{D}_0}{4} + \mathcal{D}_1 \right), \quad (4.6)$$

$$\begin{aligned} Y_2^+(x) = & C_A C_F \left(\mathcal{D}_0 \left[\frac{\zeta_3}{4} + \frac{17\pi^2}{72} - \frac{905}{288} \right] + \mathcal{D}_1 \left[\frac{95}{144} + \frac{\pi^2}{12} \right] + \frac{11\mathcal{D}_2}{8} \right) \\ & + C_F^2 \left(\mathcal{D}_0 \left[-\frac{\zeta_3}{2} + \frac{5\pi^2}{12} + \frac{67}{32} \right] + \mathcal{D}_1 \left[\frac{69}{16} + \frac{\pi^2}{6} \right] + \frac{21\mathcal{D}_2}{8} + \frac{\mathcal{D}_3}{2} \right) \\ & + C_F T_F n_l \left(\mathcal{D}_0 \left[\frac{85}{72} - \frac{\pi^2}{18} \right] - \frac{13\mathcal{D}_1}{36} - \frac{\mathcal{D}_2}{2} \right), \end{aligned} \quad (4.7)$$

$$\begin{aligned} Y_3^+(x) = & C_A C_F T_F n_l \left(\mathcal{D}_0 \left[-\frac{11\zeta_3}{18} + \frac{19\pi^4}{720} - \frac{619\pi^2}{648} + \frac{4205}{648} \right] + \mathcal{D}_1 \left[-\frac{\zeta_3}{6} + \frac{2\pi^2}{9} - \frac{5399}{1296} \right] \right. \\ & + \mathcal{D}_2 \left[\frac{\pi^2}{12} - \frac{10}{9} \right] + \frac{77}{54} \mathcal{D}_3 \Big) + C_F^2 T_F n_l \left(\mathcal{D}_1 \left[\frac{2\zeta_3}{3} - \frac{47\pi^2}{108} - \frac{1025}{216} \right] + \mathcal{D}_0 \left[\frac{37\zeta_3}{18} + \frac{\pi^4}{1080} \right. \right. \\ & - \frac{1063\pi^2}{864} - \frac{727}{432} \Big] - \frac{55}{96} \mathcal{D}_2 + \frac{55}{36} \mathcal{D}_3 + \frac{5}{12} \mathcal{D}_4 \Big) + C_F T_F^2 n_l^2 \left(\mathcal{D}_0 \left[\frac{29\pi^2}{324} - \frac{581}{648} \right] \right. \\ & + \mathcal{D}_1 \left[\frac{275}{324} - \frac{\pi^2}{27} \right] + \frac{1}{36} \mathcal{D}_2 - \frac{7}{27} \mathcal{D}_3 \Big) + N_c^3 \left(-\frac{1}{64} \mathcal{D}_5 - \frac{325}{768} \mathcal{D}_4 + \mathcal{D}_3 \left[-\frac{8323}{3456} - \frac{\pi^2}{48} \right] \right. \\ & + \mathcal{D}_2 \left[-\frac{\zeta_3}{8} - \frac{43\pi^2}{192} + \frac{6293}{9216} \right] + \mathcal{D}_1 \left[\frac{\zeta_3}{48} - \frac{101\pi^4}{5760} + \frac{55\pi^2}{2304} + \frac{221909}{41472} \right] \\ & + \mathcal{D}_0 \left[-\frac{1}{24} \pi^2 \zeta_3 + \frac{31\zeta_3}{192} - \frac{\zeta_5}{8} - \frac{4673\pi^4}{69120} + \frac{147241\pi^2}{82944} - \frac{397315}{165888} \right] \Big) \\ & + \mathcal{O}(N_c^2, n_h), \end{aligned} \quad (4.8)$$

with $\mathcal{D}_i = \left[\ln^i(1-x)/(1-x) \right]_+$. The formulae for the regular parts are rather lengthy and given in appendix B. In figure 2 we show the normalized spectrum as a function of x in the pole scheme. This extends figure 1 of ref. [25] to N³LO. The plots have been obtained by using the expansions around $x = 0$ and $x = 1$, which are available in the supplementary files to this paper. The third-order corrections amount to approximately 50% of the NNLO corrections and have the opposite sign. We refrain from performing a scheme transformation for the spectrum since it is to a large extent dominated by the singularity for $x \rightarrow 1$. Instead, we will discuss in the following subsection the total decay rate Γ_{77} , which is obtained by integrating over the photon energy.

4.2 Total rate in different renormalization schemes

We obtain the total decay rate by analytically integrating over the spectrum and expressing the occurring iterated integrals at argument 1 in terms of transcendental constants, as described in section 3.

If we choose the on-shell scheme for the bottom quark mass, the O_7 contribution to the total rate for the decay $b \rightarrow X_s \gamma$ can be cast in the form

$$\Gamma_{77} = \Gamma_0 m_b^3 \bar{m}_b^2(m_b) |C_7(m_b)|^2 \left[1 + \frac{\alpha_s}{\pi} X_1 + \left(\frac{\alpha_s}{\pi} \right)^2 X_2 + \left(\frac{\alpha_s}{\pi} \right)^3 X_3 \right]. \quad (4.9)$$

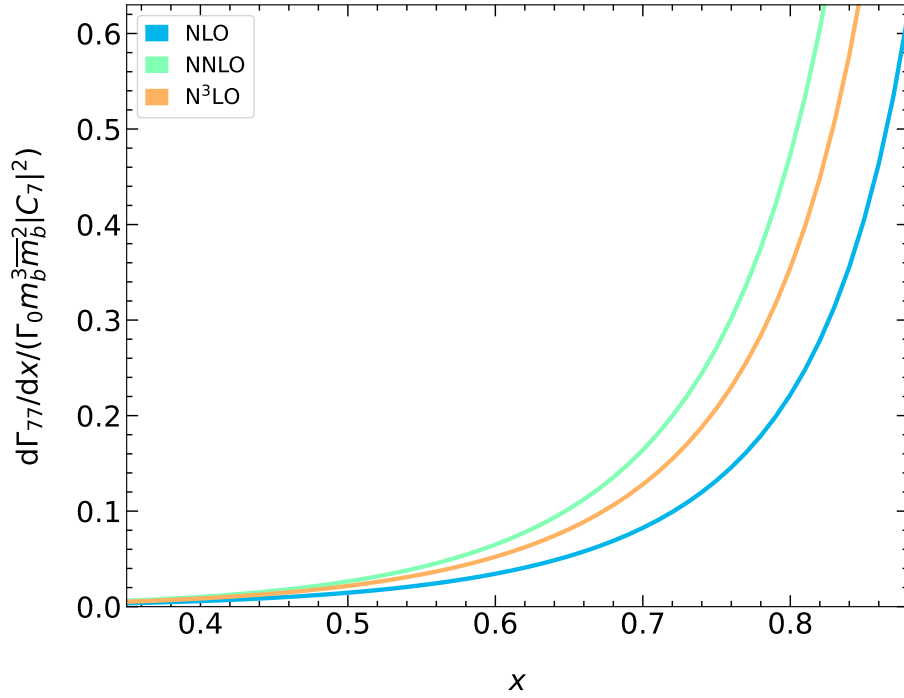


Figure 2. Normalized spectrum as a function of $x = 2E_\gamma/m_b$ in the on-shell scheme. For this plot a fixed value $\alpha_s = 0.22$ has been chosen.

Since the plus distributions integrate to zero for the decay rate, the coefficients X_i are obtained by

$$X_i = \int_0^1 dx Y_i = Y_i^\delta + \int_0^1 dx Y_i^{\text{reg}}. \quad (4.10)$$

For $\mu = m_b$ we have

$$X_1 = C_F \left(\frac{4}{3} - \frac{\pi^2}{3} \right), \quad (4.11)$$

$$\begin{aligned} X_2 = & n_l T_F C_F \left(-\frac{251}{432} + \frac{8\pi^2}{27} + \zeta_3 \right) + n_h T_F C_F \left(+\frac{3563}{648} - \frac{29\pi^2}{54} - \frac{\zeta_3}{3} \right) \\ & + C_A C_F \left(-\frac{1333}{3456} + \frac{119\pi^2}{1728} - \frac{47\zeta_3}{96} - \frac{27}{16}\pi^2 \log(2) + \frac{43\pi^4}{1440} \right) \\ & + C_F^2 \left(\frac{2825}{288} - \frac{319\pi^2}{96} - \frac{217\zeta_3}{48} + \frac{27}{8}\pi^2 \log(2) + \frac{53\pi^4}{720} \right), \end{aligned} \quad (4.12)$$

$$\begin{aligned} X_3 = & N_c^3 \left(\frac{5678117}{373248} - \frac{305723\pi^2}{62208} - \frac{13177\zeta_3}{864} + \frac{3017\pi^4}{10368} + \frac{7\pi^2\zeta_3}{72} + \frac{925\zeta_5}{96} - \frac{1271\pi^6}{181440} - \frac{3\zeta_3^2}{32} \right) \\ & + n_l^2 C_F T_F^2 \left(\frac{5519}{11664} - \frac{121\pi^2}{243} + \frac{14\zeta_3}{27} - \frac{8\pi^4}{405} \right) - n_h^2 C_F T_F^2 \left(\frac{374}{81} - \frac{2\pi^2}{15} - \frac{26\zeta_3}{9} + \frac{\pi^4}{270} \right) \end{aligned}$$

$$\begin{aligned}
 & + n_l n_h T_F^2 C_F \left(-\frac{557}{3888} - \frac{505\pi}{216\sqrt{3}} + \frac{469\pi^2}{729} - \frac{800\zeta_3}{81} - \frac{256\pi^3}{243\sqrt{3}} - \frac{7\pi^4}{2430} + \frac{128\pi\psi^{(1)}\left(\frac{1}{3}\right)}{81\sqrt{3}} \right) \\
 & + n_l T_F C_A C_F \left(-\frac{c_1}{12} - \frac{19c_2}{36} - \frac{c_3}{3} + \frac{2}{15}\pi \text{Im} \left(\text{Li}_3 \left(\frac{i}{\sqrt{3}} \right) \right) - \frac{70\text{Li}_4\left(\frac{1}{2}\right)}{9} - \frac{10187\zeta_5}{2592} \right. \\
 & - \frac{487\pi^2\zeta_3}{2592} + \frac{5\pi\zeta_3}{24\sqrt{3}} + \frac{433\zeta_3}{192} + \frac{5\pi^5}{729\sqrt{3}} + \frac{1495\pi^4}{11664} + \frac{655\pi^3}{648\sqrt{3}} + \frac{28081\pi^2}{15552} + \frac{661\pi}{576\sqrt{3}} \\
 & - \frac{1269163}{373248} - \frac{35\log^4(2)}{108} - \frac{1}{360}\pi^2\log^2(3) - \frac{395\pi^2\log^2(2)}{1296} - \frac{19\pi\log^2(2)}{72\sqrt{3}} + \frac{19\log^2(2)}{192} \\
 & - \frac{\pi^3\log(3)}{54\sqrt{3}} + \frac{\pi\log(3)}{24\sqrt{3}} + \frac{253}{72}\pi^2\log(2) - \frac{\pi\psi^{(3)}\left(\frac{2}{3}\right)}{324\sqrt{3}} - \frac{\psi^{(1)}\left(\frac{1}{3}\right)^2}{108} + \frac{\pi^3\psi^{(1)}\left(\frac{1}{3}\right)}{486\sqrt{3}} \\
 & + \frac{1}{81}\pi^2\psi^{(1)}\left(\frac{1}{3}\right) - \frac{629\pi\psi^{(1)}\left(\frac{1}{3}\right)}{432\sqrt{3}} - \frac{\psi^{(1)}\left(\frac{1}{3}\right)}{36} + \frac{\pi\log(3)\psi^{(1)}\left(\frac{1}{3}\right)}{36\sqrt{3}} \Big) \\
 & + n_l T_F C_F^2 \left(\frac{c_1}{6} + \frac{19c_2}{18} + \frac{2c_3}{3} - \frac{4}{15}\pi \text{Im} \left(\text{Li}_3 \left(\frac{i}{\sqrt{3}} \right) \right) + \frac{140\text{Li}_4\left(\frac{1}{2}\right)}{9} - \frac{613\zeta_5}{1296} \right. \\
 & + \frac{127\pi^2\zeta_3}{1296} - \frac{5\pi\zeta_3}{12\sqrt{3}} + \frac{7795\zeta_3}{864} - \frac{10\pi^5}{729\sqrt{3}} - \frac{3599\pi^4}{7290} - \frac{655\pi^3}{324\sqrt{3}} + \frac{29\pi^2}{4} - \frac{661\pi}{288\sqrt{3}} \\
 & - \frac{274397}{20736} + \frac{35\log^4(2)}{54} + \frac{1}{180}\pi^2\log^2(3) + \frac{395}{648}\pi^2\log^2(2) + \frac{19\pi\log^2(2)}{36\sqrt{3}} - \frac{19\log^2(2)}{96} \\
 & + \frac{\pi^3\log(3)}{27\sqrt{3}} - \frac{\pi\log(3)}{12\sqrt{3}} - \frac{253}{36}\pi^2\log(2) + \frac{\pi\psi^{(3)}\left(\frac{2}{3}\right)}{162\sqrt{3}} + \frac{\psi^{(1)}\left(\frac{1}{3}\right)^2}{54} - \frac{\pi^3\psi^{(1)}\left(\frac{1}{3}\right)}{243\sqrt{3}} \\
 & - \frac{2}{81}\pi^2\psi^{(1)}\left(\frac{1}{3}\right) + \frac{629\pi\psi^{(1)}\left(\frac{1}{3}\right)}{216\sqrt{3}} + \frac{\psi^{(1)}\left(\frac{1}{3}\right)}{18} - \frac{\pi\log(3)\psi^{(1)}\left(\frac{1}{3}\right)}{18\sqrt{3}} \Big) + O(N_c^2, n_h). \quad (4.13)
 \end{aligned}$$

The results for X_1 and X_2 are in agreement with ref. [96]; the result for X_3 is new. Computer-readable expressions for general renormalization scale μ can be found in the supplementary files.

The numerical evaluation for $\mu = m_b$ leads to

$$\begin{aligned}
 \Gamma_{77} = & \Gamma_0 m_b^3 \overline{m}_b^2(m_b) |C_7(m_b)|^2 \left[1 - 2.60871 \left(\frac{\alpha_s}{\pi} \right) \right. \\
 & + \left(\frac{\alpha_s}{\pi} \right)^2 \left(-32.4531 - 0.135048 n_h + 2.36358 n_l \right) \\
 & + \left(\frac{\alpha_s}{\pi} \right)^3 \left(-513.126 - 0.0631674 n_h^2 + 69.174 n_l - 0.0365688 n_h n_l - 1.91406 n_l^2 \right. \\
 & \left. \left. + \mathcal{O}(N_c^2, n_h) \right) \right] \\
 \stackrel{n_l=4, n_h=1}{=} & \Gamma_0(m_b^3 \overline{m}_b^2(m_b)) |C_7(m_b)|^2 \left[1 - 2.61 \frac{\alpha_s}{\pi} - 23.13 \left(\frac{\alpha_s}{\pi} \right)^2 - 267.26 \left(\frac{\alpha_s}{\pi} \right)^3 \right], \quad (4.14)
 \end{aligned}$$

which manifests the usual poor convergence of the perturbative series in the on-shell scheme.

One caveat of our calculation lies in the fact that we have only computed the large- N_c , light-fermion, and n_h^2 contributions. One can therefore ask if the subleading- N_c terms could partially cancel the large N³LO contributions observed here. At NNLO this does not seem to be the case. Naively the subleading- N_c terms come with a suppression factor $1/N_c$ and therefore contribute a $\sim 30\%$ shift. In practice we rather observe a correction of about 10%. We therefore do not expect the subleading- N_c terms to substantially alter the observations in this and the following sections.

In the following, we investigate the convergence and scale dependence of the total rate in the kinetic [97] and the MSR schemes [98, 99].

Kinetic scheme. We transform the pole mass $m_b \equiv m_b^{\text{pole}}$ to the kinetic scheme and we take into account the power-suppressed leading-order contributions to Γ_{77} stemming from μ_π^2 and ρ_D^3 (see for instance ref. [1]). Their transformation to the kinetic scheme induces perturbative contributions which we have to take into account. We use the conversion formula between m_b^{pole} and m_b^{kin} and the expressions for $\mu_\pi^2|_{\text{pert}}$ and $\rho_D^3|_{\text{pert}}$ up to third order from refs. [100–102]. We use the formulae from ref. [102], which correspond to massless charm quarks, as this is the approximation which we also use in the calculation of the photon spectrum. Therefore, to convert the on-shell mass to the kinetic mass we consider the expressions in appendix A of ref. [102] with $n_l = 4$ and $\alpha_s^{(4)}$ and apply the decoupling relation to express the mass relation in terms of $\alpha_s^{(5)}$. For the decoupling scale we use $\bar{m}_b(\mu)$. Converting only the on-shell mass to the kinetic scheme and reexpanding up to third order, we obtain with $m_b^{\text{kin}}(1 \text{ GeV}) = 4.55 \text{ GeV}$ and $\bar{m}_b(m_b^{\text{kin}}) = 4.14 \text{ GeV}$

$$\begin{aligned} \Gamma_{77} &= \Gamma_0 |C_7(m_b^{\text{kin}})|^2 (m_b^{\text{kin}})^3 \bar{m}_b^2(m_b^{\text{kin}}) \left[1 - 1.29 \frac{\alpha_s}{\pi} - 8.75 \left(\frac{\alpha_s}{\pi} \right)^2 - 80.82 \left(\frac{\alpha_s}{\pi} \right)^3 \right] \\ &= \Gamma_0 |C_7(m_b^{\text{kin}})|^2 (m_b^{\text{kin}})^3 \bar{m}_b^2(m_b^{\text{kin}}) \left[1 - 0.090_{\alpha_s} - 0.043_{\alpha_s^2} - 0.028_{\alpha_s^3} \right], \end{aligned} \quad (4.15)$$

where $\alpha_s \equiv \alpha_s^{(5)}(m_b^{\text{kin}})$. We observe a reasonable behaviour of the perturbative series, although with NNLO and N³LO effects still in the range of a few percent, beyond the sub-percent effect that one would naively expect.

In a next step we transform all instances of $\bar{m}_b^2$ to the kinetic scheme using the expressions from ref. [102] and obtain

$$\Gamma_{77} = \Gamma_0 |C_7(m_b^{\text{kin}})|^2 (m_b^{\text{kin}})^5 \left[1 - 3.11 \frac{\alpha_s}{\pi} - 17.13 \left(\frac{\alpha_s}{\pi} \right)^2 - 122.22 \left(\frac{\alpha_s}{\pi} \right)^3 \right]. \quad (4.16)$$

The comparison to eq. (4.15) shows that the perturbative expansion is somewhat worse, although it is still better than in the pole scheme, see eq. (4.14).

To study the dependence of the N³LO total rate on the renormalization scale μ ,² one would in principle require the evolution of the Wilson coefficient $C_7(\mu)$ at N³LL accuracy. However, the mixing between O_7 and O_8 is currently known only up to NNLL [36, 103], as is the mixing of current-current and penguin operators into O_7 and O_8 [37]. Moreover, the matching conditions are available only up to $O(\alpha_s^2)$ [34]. As a consequence, any estimate of the

²We evaluate $\alpha_s(\mu)$, $\bar{m}(\mu)$, and $C_7(\mu)$ at the same scale.

renormalization-scale uncertainty would not be limited by our N³LO evaluation of the matrix element, but by the incomplete knowledge of the running and matching of the operator O_7 .

We therefore adopt a simplified approach. We evaluate the Wilson coefficient C_7 at the scale $\mu = m_b$ and study the scale dependence of the rate by assuming that the evolution of

$$C_T(\mu) = C_7(\mu)\overline{m}_b(\mu) \quad (4.17)$$

is governed solely by the anomalous dimension of the tensor current, known up to $O(\alpha_s^4)$ from refs. [104–106].³ The μ dependence of C_T is given by the solution of the renormalization group equation

$$\mu \frac{dC_T(\mu)}{d\mu} = \gamma_T(\alpha_s)C_T(\mu), \quad (4.18)$$

which reads

$$C_T(\mu) = C_T(\mu_0) \exp \left[\int_{\alpha_s(\mu_0)}^{\alpha_s(\mu)} \frac{\gamma_T(\alpha_s)}{2\beta(\alpha_s)} d\alpha_s \right] \quad (4.19)$$

with the QCD beta function and the anomalous dimension of the tensor current given by

$$\beta(\alpha_s) = - \sum_{n=0} \beta_n \left(\frac{\alpha_s}{\pi} \right)^{n+2}, \quad \gamma_T(\alpha_s) = \sum_{n=0} \gamma_n \left(\frac{\alpha_s}{\pi} \right)^{n+1}. \quad (4.20)$$

Inserting the expansions for $\gamma_T(\alpha_s)$ and $\beta(\alpha_s)$ into eq. (4.19) and expanding in α_s gives:

$$C_T(\mu) = C_T(\mu_0) \left[1 + J_1 \frac{\alpha_s(\mu)}{\pi} + J_2 \left(\frac{\alpha_s(\mu)}{\pi} \right)^2 + J_3 \left(\frac{\alpha_s(\mu)}{\pi} \right)^3 \right] \left(\frac{\alpha_s(\mu_0)}{\alpha_s(\mu)} \right)^{\frac{\gamma_0}{2\beta_0}} \\ \times \left[1 - J_1 \frac{\alpha_s(\mu_0)}{\pi} - (J_2 - J_1^2) \left(\frac{\alpha_s(\mu_0)}{\pi} \right)^2 - (J_3 + J_1^3 - 2J_1J_2) \left(\frac{\alpha_s(\mu_0)}{\pi} \right)^3 \right], \quad (4.21)$$

where

$$J_1 = \frac{\beta_1\gamma_0}{2\beta_0^2} - \frac{\gamma_1}{2\beta_0}, \\ J_2 = \frac{\beta_1^2\gamma_0^2}{8\beta_0^4} - \frac{\beta_1^2\gamma_0}{4\beta_0^3} - \frac{\beta_1\gamma_0\gamma_1}{4\beta_0^3} + \frac{\beta_1\gamma_1}{4\beta_0^2} + \frac{\gamma_1^2}{8\beta_0^2} + \frac{\beta_2\gamma_0}{4\beta_0^2} - \frac{\gamma_2}{4\beta_0}, \\ J_3 = \frac{\beta_1^3\gamma_0^3}{48\beta_0^6} - \frac{\beta_1^3\gamma_0^2}{8\beta_0^5} + \frac{\beta_1^3\gamma_0}{6\beta_0^4} - \frac{\beta_1^2\gamma_0^2\gamma_1}{16\beta_0^5} + \frac{\beta_1^2\gamma_0\gamma_1}{4\beta_0^4} - \frac{\beta_1^2\gamma_1}{6\beta_0^3} + \frac{\beta_2\beta_1\gamma_0^2}{8\beta_0^4} + \frac{\beta_1\gamma_0\gamma_1^2}{16\beta_0^4} - \frac{\beta_1\gamma_1^2}{8\beta_0^3} \\ - \frac{\beta_2\beta_1\gamma_0}{3\beta_0^3} - \frac{\beta_1\gamma_0\gamma_2}{8\beta_0^3} + \frac{\beta_1\gamma_2}{6\beta_0^2} - \frac{\gamma_1^3}{48\beta_0^3} + \frac{\beta_3\gamma_0}{6\beta_0^2} + \frac{\beta_2\gamma_1}{6\beta_0^2} - \frac{\beta_2\gamma_0\gamma_1}{8\beta_0^3} + \frac{\gamma_1\gamma_2}{8\beta_0^2} - \frac{\gamma_3}{6\beta_0}. \quad (4.22)$$

In figure 3 we present the total decay rate in the kinetic scheme as a function of the renormalization scale μ . Specifically, we consider the rate Γ_{77} normalized to $C_T^2 = |C_7|^2 \overline{m}_b^2$, evaluated at the reference scale $\mu = m_b^{\text{kin}}$, and to an additional mass factor $(m_b^{\text{kin}})^3$. With this normalization, the dependence of the rate on μ can be studied without fixing the numerical value of $C_7(m_b^{\text{kin}})$.

³Eq. (3.2) of ref. [106] contains a typo: the colour factor $d_A^{abcd}d_A^{abcd}$ at order α_s^4 must be replaced by $N_F d_F^{abcd}d_F^{abcd}$ to have agreement with ref. [105].

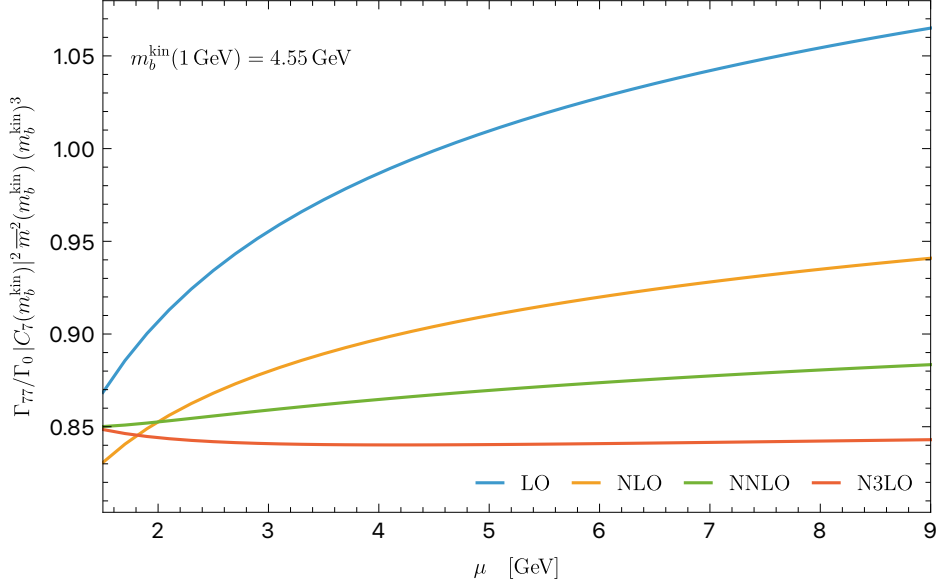


Figure 3. The total partonic decay rate in the kinetic mass scheme as a function of the renormalization scale μ .

The N^n LO curves are obtained by multiplying our result for the matrix element up to α_s^n , evaluated at the scale μ , by $C_T(\mu)$ as given in eq. (4.21) considering the RGE resummation up to N^n LL, without reexpanding the result in α_s . For the numerical evaluation of $\alpha_s^{(5)}(\mu)$ and $\bar{m}_b(\mu)$ we employ RunDec [107, 108], using $\alpha_s^{(5)}(M_Z) = 0.118$ and $\bar{m}_b^{(5)}(\bar{m}_b) = 4.2$ GeV as input values.

Over the entire range $m_b^{\text{kin}}/2 \leq \mu < 2m_b^{\text{kin}}$, the sensitivity of the rate to the renormalization scale is progressively reduced with the inclusion of higher-order corrections. The 7% variation observed at leading order decreases to 4%, 1.5%, and 0.2% upon including NLO, NNLO, and N^3 LO corrections in the matrix element and in the running, respectively. On the other hand, we find only a marginal overlap of the uncertainty bands obtained from a simple variation of μ . In particular, the N^3 LO prediction does not overlap with the NNLO error band for $m_b^{\text{kin}}/2 \leq \mu < 2m_b^{\text{kin}}$. As a consequence, the NNLO uncertainty band obtained from scale variation does not fully account for the size of the genuine higher-order contributions, indicating that, at NNLO, the μ variation by a factor 2 underestimates the impact of missing perturbative corrections in this observable.

MSR scheme. As an alternative to the kinetic mass scheme we transform the pole mass into the MSR scheme. We follow ref. [99] and use the so-called “practical MSR” mass, which is introduced in section 2.3 of that reference.

With $\mu_s = m_b^{\text{MSR}}$, $m_b^{\text{MSR}}(1 \text{ GeV}) = 4.66$ GeV, and $\bar{m}_b(m_b^{\text{MSR}}) = 4.122$ GeV we obtain

$$\begin{aligned} \Gamma_{77} &= \Gamma_0 |C_7(m_b^{\text{MSR}})|^2 (m_b^{\text{MSR}})^3 \bar{m}_b^2(\mu_s) \left[1 - 1.75 \frac{\alpha_s}{\pi} - 13.30 \left(\frac{\alpha_s}{\pi} \right)^2 - 121.50 \left(\frac{\alpha_s}{\pi} \right)^3 \right] \\ &= \Gamma_0 |C_7(m_b^{\text{MSR}})|^2 (m_b^{\text{MSR}})^3 \bar{m}_b^2(\mu_s) \left[1 - 0.121 \alpha_s - 0.064 \alpha_s^2 - 0.040 \alpha_s^3 \right]. \end{aligned} \quad (4.23)$$

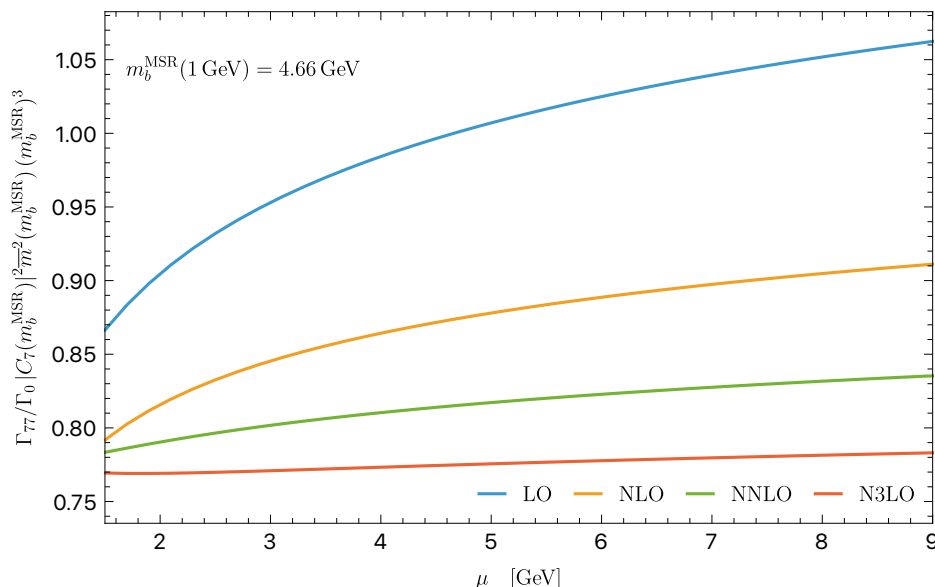


Figure 4. The total partonic decay rate with m_b in the MSR scheme as a function of the renormalization scale μ .

Also for this MSR scheme we observe a reasonable behaviour of the perturbative series, although with larger corrections as in the kinetic mass scheme, see eq. (4.15). Following the same approach as the kinetic scheme, we show in figure 4 the dependence of the rate on μ in the range $m_b^{\text{MSR}}/2 \leq \mu \leq 2m_b^{\text{MSR}}$. Also in this case we observe a reduction of the 7% scale uncertainty of the LO. The inclusion of NLO, NNLO, and N³LO corrections reduces the uncertainty based on scale variation to 4%, 2%, and 0.7%. However, again the size of the higher-order corrections is not captured by this simple estimate.

4.3 Branching ratio with photon energy cut

When integrating over the spectrum, it is possible to introduce a lower cut on the photon energy and define the cut-dependent integrated decay rate as

$$\Gamma(E_{\text{cut}}) = \int_{E_{\text{cut}}}^{m_b/2} \frac{d\Gamma}{dE} dE. \quad (4.24)$$

For $E_{\text{cut}} = 0$ we obtain the results presented in section 4.2. If $E_{\text{cut}} > 0$, it is convenient to split the integrand in eq. (4.24) into the singular and regular part. The former gets contributions from the δ functions which is identical for all values of E_{cut} . This part can be taken over from section 4.2. For the contribution of the plus distributions to the singular part one has to take care of the fact that for the lower bound of the integral in eq. (4.24) we have $E_{\text{cut}} > 0$. This leads to an additional term which can be expressed as an integral over the region $E \in [0, E_{\text{cut}}]$ where the plus distributions are regular, see eq. (A.4). This contribution contains an explicit dependence on the bottom quark mass, even from the integration boundary, which has to be taken into account when performing scheme changes. This is also the case for the regular part.

E_{cut}	X_1^{cut}	X_2^{cut}	X_3^{cut}	$\Gamma_{77}^{\text{norm}}$
0.5 GeV	−1.2909	−8.75	−80.84	0.840
1.0 GeV	−1.3016	−8.81	−81.27	0.839
1.6 GeV	−1.4264	−9.56	−87.42	0.824
1.8 GeV	−1.5939	−10.55	−9.613	0.805
2.0 GeV	−2.0434	−12.84	−117.14	0.755
2.2 GeV	−4.2763	−11.28	−155.90	0.594

Table 1. Coefficients of the perturbative expansion of $\Gamma_{77}(E_{\text{cut}})$ in the kinetic scheme, keeping the factor $\bar{m}_b^2$. The LO contribution is independent on E_{cut} and always equal to one. $\Gamma_{77}^{\text{norm}}$ is defined such that the factor $\Gamma_0|C_7(m_b^{\text{kin}})|^2 (m_b^{\text{kin}})^3 \bar{m}_b^2(m_b^{\text{kin}})$ is divided out. For the renormalization scale we have chosen $\mu = m_b^{\text{kin}}$.

E_{cut}	X_1^{cut}	X_2^{cut}	X_3^{cut}	$\Gamma_{77}^{\text{norm}}$
0.5 GeV	−1.7508	−13.31	−121.52	0.775
1.0 GeV	−1.7603	−13.36	−121.95	0.774
1.6 GeV	−1.8676	−14.06	−128.04	0.761
1.8 GeV	−2.0050	−14.97	−136.86	0.744
2.0 GeV	−2.3468	−17.19	−159.69	0.702
2.2 GeV	−3.6149	−23.31	−225.13	0.563

Table 2. Coefficients of the perturbative expansion of $\Gamma_{77}(E_{\text{cut}})$ in the MSR scheme. The LO contribution is independent on E_{cut} and always equal to one. $\Gamma_{77}^{\text{norm}}$ is defined such that the factor $\Gamma_0|C_7(m_b^{\text{MSR}})|^2 (m_b^{\text{MSR}})^3 \bar{m}_b^2(m_b^{\text{MSR}})$ is divided out. For the renormalization scale we have chosen $\mu = m_b^{\text{MSR}}$.

It is convenient to define

$$X_i^{\text{cut}} = \int_{x_{\text{cut}}}^1 dx Y_i \quad (4.25)$$

with $x_{\text{cut}} = 2E_{\text{cut}}/m_b$ such that the E_{cut} -dependent integrated decay rate is given by

$$\Gamma_{77}(E_{\text{cut}}) = \Gamma_0|C_7(m_b)|^2 m_b^3 \bar{m}_b^2(m_b) \left[1 + \sum_{i=1}^3 \left(\frac{\alpha_s}{\pi} \right)^i X_i^{\text{cut}} \right]. \quad (4.26)$$

Our results are shown in tables 1 and 2 for the kinetic (keeping the factor $\bar{m}_b^2$) and MSR schemes, respectively, for various values of E_{cut} . We observe a similar pattern as in section 4.2: NLO, NNLO, and N³LO corrections have the same sign and are negative. Figure 5 shows the properly normalized decay rate Γ_{77} as a function of E_{cut} .

4.4 Comparison to previous estimates of the N³LO corrections

In ref. [23] the photon energy spectrum has been analysed by matching resummed singular contributions in the peak region, i.e. for large values of the photon energy, to fixed order results in the tail region. In this analysis a couple of fixed-order three-loop contributions were

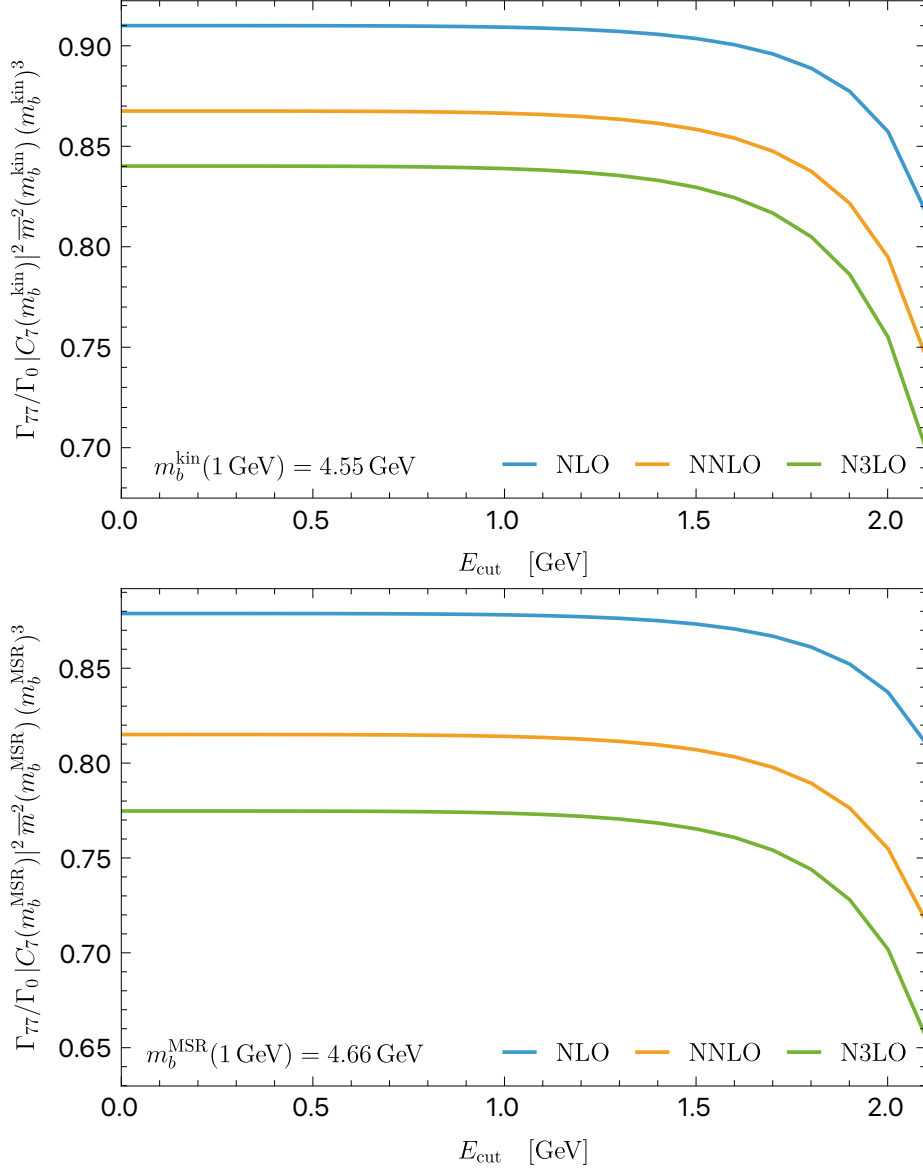


Figure 5. The O_7 contribution to the rate Γ as a function of on the lower cut on the photon energy E_{cut} in the kinetic scheme (top) and the MSR scheme (bottom).

not known explicitly, but treated as nuisance parameters in the fit to data. In particular, the following two ingredients were unavailable:

- The finite part of the three-loop heavy-to-light form factor, which has been computed in ref. [24].
- The finite part of the three-loop $b \rightarrow s\gamma$ spectrum $Y_3(x)$, which is computed in this paper in the large- N_c limit, including all light-fermion and n_h^2 contributions.

In ref. [24] it was shown that the three-loop contribution to the heavy-to-light form factor is significantly larger than the estimate used in the ref. [23]:

$$h_3^{\text{Ref. [23]}} = 0 \pm 80, \quad h_3^{\text{exact}} = -181.1617381 \dots \quad (4.27)$$

With the calculation presented in this work we are in a position to address also the second unknown ingredient. In ref. [23] the contribution to $Y_3(x)$ is split into a singular and a regular piece,

$$Y_3(x) = Y_3^{\text{sing}}(x) + Y_3^{\text{reg}}(x).$$

The singular piece consists of all distributions and can be calculated within SCET from known ingredients. In ref. [23] the expression is given for SU(3) and we agree with the one- and two-loop expressions. At three loops we can only compare the terms proportional to powers of n_1 and we find agreement as well.

In ref. [23] the prediction for the regular contribution $Y_3^{\text{reg}}(x)$ was done for an effective Wilson coefficient, including contributions from the Wilson coefficients of other operators besides O_7 considered in the present paper. Hence, a direct comparison is not possible. Instead, we follow the same prescription to derive an estimate for our expression: The regular piece is split into

$$Y_3^{\text{reg}}(x) = Y_3^{\text{corr}} + Y_3^{\text{uncorr}}(x), \quad (4.28)$$

with $Y_3^{\text{corr}} = -Y_3^{\text{sing}}(0)$. This ensures that $Y_3^{\text{uncorr}}(0) = 0$ [23]. $Y_3^{\text{uncorr}}(x)$ is then modelled via powers of the analytically known spectrum at NLO, $Y_1(x)$, via

$$Y_3^{\text{uncorr}}(x) = \sum_{i=0}^5 c_i \left(\frac{Y_1(x) - Y_1(0)}{4} \right)^i, \quad (4.29)$$

with $\max(|c_i|)$ taken to be $\{20, 100, 80, 10, 5, 1\}$. This ensures that the powers of logarithms in the limit $x \rightarrow 1$ are reproduced correctly. The uncertainty around the central value 0 is then obtained by varying the six parameters independently and adding the corresponding uncertainties in quadrature. In figure 6 we show the region covered by this ansatz as well as our leading-color, light-fermion, and n_h^2 result for $Y_3^{\text{uncorr}}(x)$. We notice that the ansatz provides a decent estimate of the corrections, albeit slightly underestimating the uncertainty. However, especially in the limit $x \rightarrow 1$ the uncertainties become large. With the results obtained in the present paper, we are able to shrink them significantly to the missing sub-leading color contributions only.

5 Conclusions

In this work we consider the photon energy spectrum of the partonic radiative decay $b \rightarrow X_s \gamma$, induced by the electric dipole operator O_7 . We reproduce the NNLO results available in the literature and compute all light-fermion and n_h^2 contributions as well as the leading term in the large- N_c expansion at N³LO.

In our approach, we compute the imaginary part of the forward scattering amplitude $b\gamma \rightarrow b\gamma$, which must be considered up to three loops. Since the spectrum is divergent at the end point, i.e., for $E_\gamma \rightarrow m_b/2$, it is important to distinguish the individual branches during the computation, which we realize at the level of the master integrals. This allows us to isolate the singular behaviour and write the analytic expressions in terms of δ and plus distributions

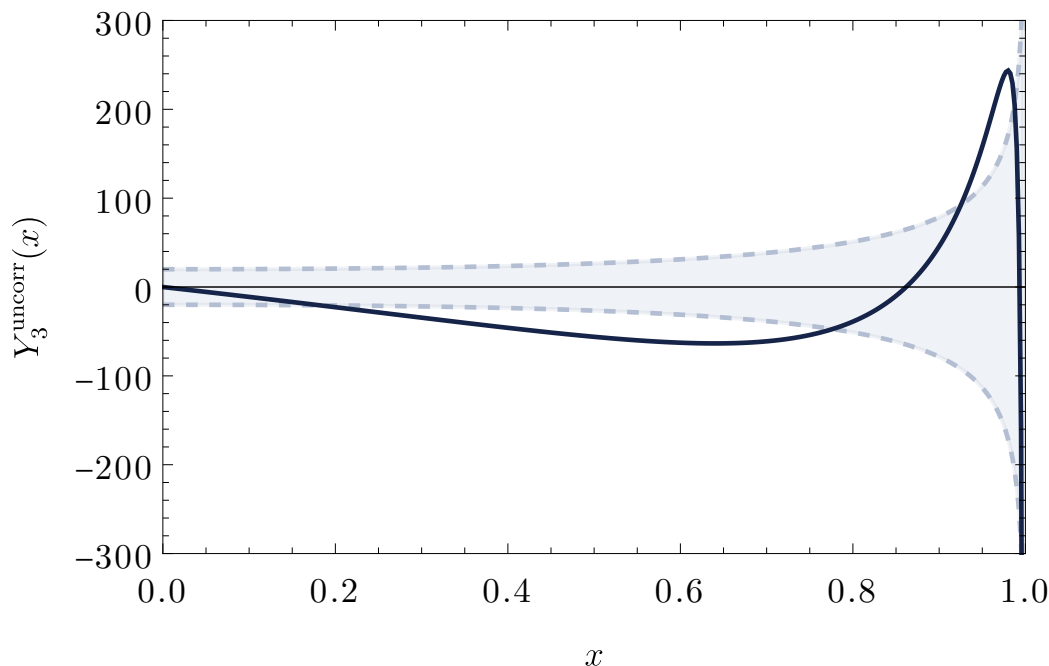


Figure 6. Comparison between the modelling of nuisance parameters related to the, at that point unknown, $Y_3^{\text{uncorr}}(x)$ following ref. [23] (gray band) and the leading-color, light-fermion, and n_h^2 results obtained in this paper (black line).

and functions which are regular for $E_\gamma \rightarrow m_b/2$. We provide explicit analytic results for the spectrum which can be downloaded in computer-readable from the supplementary files.

Analytic results for the total inclusive decay rate $\Gamma_{77}(b \rightarrow X_s \gamma)$ are obtained after integrating over all kinematically allowed values of E_γ . We discuss the convergence properties in three different renormalization schemes and observe a significant improvement after applying a short-distance scheme. We also compute the integrated decay rate as a function of the photon energy cut.

The techniques presented in this work can also be applied to the contributions from subleading colour factors. In that case, however, also non-planar Feynman diagrams contribute. Furthermore, the number of master integrals is significantly higher, which complicates analytical calculations and likely necessitates numerical methods. Our method can also be used to calculate the contribution from the chromomagnetic dipole operator O_8 to the photon energy spectrum.

Acknowledgments

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A Distributions

For the expansion into distributions we can follow ref. [111] and use

$$\int_0^1 dy \left[\frac{1}{y^m} \right]_+ f(y) = \int_0^1 \frac{dy}{y^m} \left[f(y) - \sum_{i=0}^{m-1} \frac{f^{(i)}(0)}{i!} y^i \right]. \quad (\text{A.1})$$

Specified to the cases we encounter in our calculations this leads to:

$$\begin{aligned} \int_0^1 dy \frac{f(y)}{y^{1-n\epsilon}} &= \int_0^1 dy \left[\left[y^{-1+n\epsilon} \right]_+ f(y) + \frac{1}{n\epsilon} f(0) \delta(y) \right], \\ \int_0^1 dy \frac{f(y)}{y^{2-n\epsilon}} &= \int_0^1 dy \left[\left[y^{-2+n\epsilon} \right]_+ f(y) + \left(\frac{1}{-1+n\epsilon} f(0) + \frac{1}{2n\epsilon} f'(0) \right) \delta(y) \right]. \end{aligned} \quad (\text{A.2})$$

Note that the terms in the parenthesis $[\dots]_+$ can be expanded in ϵ .

While integrals over the full phase space involving plus distributions vanish,

$$\int_0^1 dy \left[\frac{\log^i(y)}{y} \right]_+ = 0, \quad (\text{A.3})$$

integrals with a lower cut on the photon energy give the finite contribution

$$\int_0^{y_{\text{cut}}} dy \left[\frac{\log^i(y)}{y} \right]_+ = - \int_{y_{\text{cut}}}^1 dy \frac{\log^i(y)}{y} = \frac{\log^{i+1}(y_{\text{cut}})}{i+1}, \quad (\text{A.4})$$

which vanishes in the limit $y_{\text{cut}} \rightarrow 1$.

B Analytic results for the regular part of the photon spectrum

In this appendix we show the analytic results of the regular parts of the spectrum introduced in section 3 and eq. (4.1). The singular parts can be found in eqs. (4.5) and (4.8). We express the amplitude in terms of $y = 1 - x$ and use the definition of iterated integrals introduced in eq. (3.4), where we drop the argument y to shorten the expressions. The analytic expressions can be found in the supplementary material attached to this paper. At NLO and NNLO our results read

$$\begin{aligned} Y_1^{\text{reg}} &= C_F \left\{ \frac{6+3y-2y^2}{4} - \frac{(2-y)H_0}{2} \right\}, \quad (\text{B.1}) \\ Y_2^{\text{reg}} &= C_F^2 \left\{ -\frac{32+56y+413y^2-148y^3-8y^4}{96y} + \frac{H_0 P_1}{48(1-y)y} + \frac{H_{-1,0} P_2}{12(1-y)y^3} + \frac{H_{0,0} P_3}{12(1-y)} \right. \\ &\quad - \frac{H_{1,0} P_4}{12(1-y)y^3} - \frac{(2+y-y^2-y^3)H_{-1,-1,0}}{2y} + \frac{(2+y-y^2-y^3)H_{-1,0,0}}{y} \\ &\quad + \frac{(2+y-y^2-y^3)H_{-1,1,0}}{2y} + \frac{(2+y-y^2-3y^3)H_{0,-1,0}}{2y} + \frac{3(2+y-y^2-y^3)H_{0,0,0}}{2(1-y)} \\ &\quad - \frac{(1-y)(2+y)H_{0,1,0}}{2} + \frac{(2+y-y^2-y^3)H_{1,-1,0}}{2y} + \frac{(2+10y-y^2)H_{1,0,0}}{4y} \\ &\quad \left. - \frac{(2+10y-y^2)H_{1,1,0}}{4y} - \frac{(9-5y+y^2)\zeta_3}{4} + \left[\frac{P_{69}}{72(1-y)} + \frac{(2+y-y^2-y^3)H_{-1}}{24y} \right] \right\} \end{aligned}$$

$$\begin{aligned}
 & -\frac{(9+y^2)H_1}{24} + \frac{1-y-y^2}{12}H_0 \Big] \pi^2 \Big\} \\
 & + C_A C_F \Big\{ \frac{48+432y+999y^2-706y^3-12y^4}{288y} - \frac{H_0 P_5}{144(1-y)y} - \frac{H_{-1,0} P_6}{24(1-y)y^3} \\
 & + \frac{(90-24y+4y^2+y^3-y^4)H_{0,0}}{24} + \frac{H_{1,0} P_7}{24y^3} + \frac{(2+y-y^2-y^3)H_{-1,-1,0}}{4y} \\
 & - \frac{(2+y-y^2-y^3)H_{-1,0,0}}{2y} - \frac{(2+y-y^2-y^3)H_{-1,1,0}}{4y} - \frac{(2+y-y^2-3y^3)H_{0,-1,0}}{4y} \\
 & - \frac{3y^2 H_{0,0,0}}{4} + \frac{(1-y)(2+y)H_{0,1,0}}{4} - \frac{(2+y-y^2-y^3)H_{1,-1,0}}{4y} + \frac{(9-5y+y^2)\zeta_3}{8} \\
 & + \Big[\frac{P_{68}}{144(1-y)} - \frac{(2+y-y^2-y^3)H_{-1}}{48y} - \frac{(2+y-y^2-y^3)H_1}{48y} + \frac{3-y+y^2}{24}H_0 \Big] \pi^2 \Big\} \\
 & + C_F n_l T_F \Big\{ -\frac{66+21y-38y^2}{72} + \frac{(38-33y+7y^2+6y^3)H_0}{36(1-y)} - \frac{(2-y)H_{0,0}}{2} \\
 & - \frac{(2+2y-y^2)H_{1,0}}{6y} + \frac{(y-2)\pi^2}{36} \Big\}, \tag{B.2}
 \end{aligned}$$

and at N³LO we have

$$\begin{aligned}
 Y_3^{\text{reg}} = & C_F n_l^2 T_F^2 \Big\{ \frac{378-111y-406y^2}{648} - \frac{(298-225y+65y^2+114y^3)H_0}{324(1-y)} \\
 & + \frac{(26-27y+17y^2+2y^3)H_{0,0}}{18(1-y)} + \frac{(4+6y-12y^2+11y^3)H_{1,0}}{27(1-y)y} - \frac{-7(-2+y)H_{0,0,0}}{9} \\
 & - \frac{2(2+2y-y^2)H_{0,1,0}}{9y} - \frac{(2+2y-y^2)H_{1,0,0}}{3y} - \frac{(2+2y-y^2)H_{1,1,0}}{9y} \\
 & + \pi^2 \Big[\frac{2-15y+37y^2-6y^3}{324(1-y)} - \frac{(2-y)H_0}{54} - \frac{(2+2y-y^2)H_1}{54y} \Big] \Big\} \\
 & + C_F n_h n_l T_F^2 \Big\{ \frac{P_8}{2592(1-y)y^3} - \frac{H_0 P_9}{81(1-y)y^3} - \frac{(2+2y-y^2)H_1}{32y} + \frac{H_a P_{10}}{432(1-y)y^2} \\
 & + \frac{H_{1,0} P_{11}}{27(1-y)y^4} + \frac{H_{a,a} P_{12}}{216(1-y)y^4} - \frac{(2+2y-y^2)H_{b,a}}{24y} - \frac{(2+2y-y^2)H_{0,a,a}}{36y} \\
 & - \frac{(2+2y-y^2)H_{1,1,0}}{9y} - \frac{(2+2y-y^2)H_{1,a,a}}{12y} \Big\} + C_F^2 n_l T_F \Big\{ \frac{P_{13}}{27648(1-y)^2 y} \\
 & - \frac{H_0 P_{14}}{432(1-y)y} - \frac{(3008-1659y+422y^2+36y^3)H_1}{2304y} - \frac{H_a P_{15}}{288(1-y)^2 y} - \frac{H_{-1,0} P_{16}}{72(1-y)y^3} \\
 & + \frac{H_{0,0} P_{17}}{144(1-y)y} - \frac{3(6+9y-5y^2)H_{0,1}}{64y} + \frac{H_{1,0} P_{18}}{72(1-y)(2-y)y^3} - \frac{H_{a,a} P_{19}}{288(1-y)^2(2-y)y^2} \\
 & - \frac{(41-78y+33y^2+y^3)H_{b,a}}{48y} + \frac{H_{-1,-1,0} P_{20}}{18y^3} + \frac{H_{-1,0,0} P_{21}}{36(1-y)y^3} + \frac{H_{0,-1,0} P_{22}}{9(1-y)^2 y^3} \\
 & - \frac{H_{0,0,0} P_{23}}{12(1-y)(1+y)} - \frac{(10-5y-10y^2+8y^4)H_{-1,1,0}}{9(1-y)y} - \frac{H_{0,1,0} P_{24}}{18(1-y)^2 y^3} - \frac{H_{0,a,a} P_{25}}{144(1-y)^2 y} \\
 & - \frac{(6+9y-5y^2)H_{0,b,a}}{16y} - \frac{(10-5y-10y^2+8y^4)H_{1,-1,0}}{9(1-y)y} - \frac{H_{1,0,0} P_{26}}{36(1-y)y^3} \Big\}
 \end{aligned}$$

$$\begin{aligned}
 & - \frac{(118 - 129y + 48y^2 + 2y^3)H_{1,a,a}}{48y} + \frac{H_{2,1,0}P_{28}}{18(1-y)^2y} + \frac{H_{2,a,a}P_{29}}{36(1-y)^2y} \\
 & - \frac{(2+y-y^2-y^3)H_{-1,-1,-1,0}}{3y} - \frac{5(2+y-y^2-y^3)H_{-1,-1,0,0}}{6y} - \frac{H_{1,1,0}P_{27}}{36(1-y)y^3} \\
 & + \frac{(2-y^2-2y^3)H_{-1,0,-1,0}}{3y} + \frac{(2+y)(5+y-3y^2)H_{-1,0,0,0}}{2y} \\
 & + \frac{(2+3y-y^2+y^3)H_{-1,0,1,0}}{6y} + \frac{3(2+y-y^2-y^3)H_{-1,1,0,0}}{2y} \\
 & + \frac{(2+y-y^2-y^3)H_{-1,1,1,0}}{3y} - \frac{(2+y-y^2+y^3)H_{0,-1,-1,0}}{3y} \\
 & + \frac{(26+13y-13y^2-23y^3)H_{0,-1,0,0}}{6y} + \frac{2(2+y-y^2-y^3)H_{0,-1,1,0}}{3y} \\
 & + \frac{(4+3y-2y^2-3y^3)H_{0,0,-1,0}}{3y} + \frac{-5(-2+y-y^2+y^3)H_{0,0,0,0}}{(1-y)} \\
 & - \frac{(4+9y-20y^2+7y^3-y^4)H_{0,0,1,0}}{6(1-y)y} - \frac{(9-5y)H_{0,0,a,a}}{24} + \frac{2(2+y-y^2-y^3)H_{0,1,-1,0}}{3y} \\
 & - \frac{(2+9y-23y^2-2y^3+11y^4)H_{0,1,0,0}}{6(1-y)y} - \frac{(22+25y-14y^2)H_{0,1,1,0}}{6y} \\
 & - \frac{(6+9y-5y^2)H_{0,1,a,a}}{8y} + \frac{3(2+y-y^2-y^3)H_{1,-1,0,0}}{2y} + \frac{(2+y-y^2-y^3)H_{1,-1,1,0}}{3y} \\
 & + \frac{2(1+y)(2-y^2)H_{1,0,-1,0}}{3y} + \frac{(10+24y-31y^2+5y^3-4y^4)H_{1,0,0,0}}{4(1-y)y} \\
 & - \frac{(4+15y-2y^2)H_{1,0,1,0}}{6y} + \frac{(4+3y-2y^2)H_{1,0,a,a}}{24y} + \frac{(2+y-y^2-y^3)H_{1,1,-1,0}}{3y} \\
 & - \frac{(10+26y-5y^2)H_{1,1,0,0}}{6y} - \frac{(2+10y-y^2)H_{1,1,1,0}}{3y} - \frac{(4+3y-2y^2)H_{1,2,1,0}}{3y} \\
 & - \frac{(4+3y-2y^2)H_{1,2,a,a}}{6y} + \zeta_3 \left[\frac{P_{30}}{36(1-y)} - \frac{(1-y)(4+5y+3y^2)H_{-1}}{6y} \right. \\
 & + \frac{(4-6y+3y^2-2y^3)H_0}{6(1-y)} - \left. \frac{(2-17y-y^2-2y^3)H_1}{6y} \right] + \frac{(129-37y+63y^2)\pi^4}{2160} \\
 & + \pi^2 \left[\frac{P_{73}}{864y^2(1-y)} - \frac{P_{72}H_0}{216(1-y^2)} - \frac{P_{70}H_1}{216y^3(1-y)} + \frac{P_{71}H_{-1}}{216y^3(1-y)} \right. \\
 & - \frac{(2+y-y^2-y^3)H_{-1,-1}}{36y} + \frac{5(1+y^2)H_{-1,0}}{36} + \frac{(2+y-y^2-y^3)H_{-1,1}}{18y} \\
 & + \frac{(6+3y-3y^2-5y^3)H_{0,-1}}{36y} - \frac{(1+5y+y^2-4y^3)H_{0,0}}{12(1-y)} \\
 & - \frac{(12+14y-7y^2+2y^3)H_{0,1}}{36y} + \frac{(2+y-y^2-y^3)H_{1,-1}}{18y} \\
 & \left. + \frac{(2-26y-y^2-4y^3)H_{1,0}}{72y} - \frac{(2+19y-y^2+y^3)H_{1,1}}{36y} \right] \Big\} \\
 & + C_A C_F n_l T_F \left\{ \frac{P_{31}}{165888(1-y)^2y} + \frac{H_0 P_{32}}{1296(1-y)y} + \frac{(3008-1659y+422y^2+36y^3)H_1}{4608y} \right.
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{H_a P_{33}}{576(1-y)^2 y} + \frac{H_{-1,0} P_{34}}{144(1-y)y^3} - \frac{H_{0,0} P_{35}}{144(1-y)y} + \frac{3(6+9y-5y^2)H_{0,1}}{128y} \\
 & - \frac{H_{1,0} P_{36}}{432(1-y)(2-y)y^3} + \frac{H_{a,a} P_{37}}{576(1-y)^2(2-y)y^2} + \frac{(41-78y+33y^2+y^3)H_{b,a}}{96y} \\
 & - \frac{H_{-1,-1,0} P_{38}}{36y^3} - \frac{H_{-1,0,0} P_{39}}{72(1-y)y^3} + \frac{(10-5y-10y^2+8y^4)H_{-1,1,0}}{18(1-y)y} - \frac{H_{0,-1,0} P_{40}}{18(1-y)^2 y^3} \\
 & + \frac{H_{0,0,0} P_{41}}{72(1-y)(1+y)} + \frac{H_{0,1,0} P_{42}}{72(1-y)^2 y^3} + \frac{H_{0,a,a} P_{43}}{288(1-y)^2 y} + \frac{(6+9y-5y^2)H_{0,b,a}}{32y} \\
 & + \frac{(10-5y-10y^2+8y^4)H_{1,-1,0}}{18(1-y)y} + \frac{H_{1,0,0} P_{44}}{72y^3} + \frac{H_{1,1,0} P_{45}}{72y^3} - \frac{H_{2,1,0} P_{46}}{36(1-y)^2 y} \\
 & + \frac{(118-129y+48y^2+2y^3)H_{1,a,a}}{96y} + \frac{(2+y-y^2-y^3)H_{-1,-1,-1,0}}{6y} \\
 & + \frac{5(2+y-y^2-y^3)H_{-1,-1,0,0}}{12y} - \frac{(2-y^2-2y^3)H_{-1,0,-1,0}}{6y} - \frac{H_{2,a,a} P_{47}}{72(1-y)^2 y} \\
 & - \frac{(2+y)(5+y-3y^2)H_{-1,0,0,0}}{4y} - \frac{(2+3y-y^2+y^3)H_{-1,0,1,0}}{12y} \\
 & - \frac{3(2+y-y^2-y^3)H_{-1,1,0,0}}{4y} - \frac{(2+y-y^2-y^3)H_{-1,1,1,0}}{6y} - \frac{(6+7y+21y^2)\pi^4}{1440} \\
 & + \frac{(2+y-y^2+y^3)H_{0,-1,-1,0}}{6y} - \frac{(26+13y-13y^2-23y^3)H_{0,-1,0,0}}{12y} \\
 & - \frac{(2+y-y^2-y^3)H_{0,-1,1,0}}{3y} - \frac{(4+3y-2y^2-3y^3)H_{0,0,-1,0}}{6y} - \frac{5y^2 H_{0,0,0,0}}{2} \\
 & + \frac{(6+15y-6y^2+y^3)H_{0,0,1,0}}{12y} + \frac{(9-5y)H_{0,0,a,a}}{48} - \frac{(2+y-y^2-y^3)H_{0,1,-1,0}}{3y} \\
 & + \frac{(2+12y-6y^2-11y^3)H_{0,1,0,0}}{12y} + \frac{(9+11y-6y^2)H_{0,1,1,0}}{6y} + \frac{(6+9y-5y^2)H_{0,1,a,a}}{16y} \\
 & - \frac{3(2+y-y^2-y^3)H_{1,-1,0,0}}{4y} - \frac{(2+y-y^2-y^3)H_{1,-1,1,0}}{6y} - \frac{(1+y)(2-y^2)H_{1,0,-1,0}}{3y} \\
 & + \frac{(1-2y^2)H_{1,0,0,0}}{4} + \frac{H_{1,0,1,0}}{4} - \frac{(4+3y-2y^2)H_{1,0,a,a}}{48y} - \frac{(2+y-y^2-y^3)H_{1,1,-1,0}}{6y} \\
 & + \frac{(4+3y-2y^2)H_{1,2,1,0}}{6y} + \frac{(4+3y-2y^2)H_{1,2,a,a}}{12y} + \zeta_3 \left[-\frac{P_{48}}{72(1-y)} \right. \\
 & + \frac{(1-y)(4+5y+3y^2)H_{-1}}{12y} - \frac{(4+y+2y^2)H_0}{12} + \left. \frac{(8+5y-4y^2-2y^3)H_1}{12y} \right] \\
 & + \pi^2 \left[-\frac{P_{74}}{2592y^2(1-y)} - \frac{P_{75}H_0}{432(1-y^2)} + \frac{P_{76}H_1}{432y^3(1-y)} - \frac{P_{77}H_{-1}}{432y^3(1-y)} \right. \\
 & + \frac{(2+y-y^2-y^3)H_{-1,-1}}{72y} - \frac{5(1+y^2)H_{-1,0}}{72} - \frac{(2+y-y^2-y^3)H_{-1,1}}{36y} \\
 & - \frac{(6+3y-3y^2-5y^3)H_{0,-1}}{72y} + \frac{(5-2y+4y^2)H_{0,0}}{24} + \frac{(8+11y-5y^2+2y^3)H_{0,1}}{72y} \\
 & \left. - \frac{(2+y-y^2-y^3)H_{1,-1}}{36y} + \frac{(1+y^2)H_{1,0}}{36} - \frac{(2+y-y^2-y^3)H_{1,1}}{72y} \right] \Big\}
 \end{aligned}$$

$$\begin{aligned}
 & + N_c^3 \left\{ -\frac{18144 - 98460y - 57567y^2 + 625304y^3}{165888y} + \frac{H_0 P_{49}}{82944(1-y)(2-y)y} \right. \\
 & + \frac{H_{0,0} P_{50}}{4608(1-y)(2-y)^3} - \frac{H_{1,0} P_{51}}{3456(1-y)(2-y)^3 y^2} - \frac{H_{0,0,0} P_{52}}{2304(1-y)(2-y)^4} \\
 & - \frac{H_{0,1,0} P_{53}}{2304(1-y)y} - \frac{H_{1,0,0} P_{54}}{2304(1-y)(2-y)^4 y} - \frac{H_{1,1,0} P_{55}}{2304(1-y)(2-y)^4 y} - \frac{H_{0,0,0,0} P_{56}}{128(1-y)^2} \\
 & - \frac{H_{0,0,1,0} P_{57}}{384(1-y)y} - \frac{H_{0,1,0,0} P_{58}}{384(1-y)y} + \frac{H_{0,1,1,0} P_{59}}{384y} - \frac{H_{1,0,0,0} P_{60}}{128(1-y)(2-y)^5 y} + \frac{H_{1,0,1,0} P_{61}}{384(1-y)y} \\
 & + \frac{H_{1,1,0,0} P_{62}}{384(1-y)(2-y)^5 y} + \frac{H_{1,1,1,0} P_{63}}{384(1-y)(2-y)^5 y^2} - \frac{(60 - 11y - 6y^2) H_{0,0,0,0,0}}{32(1-y)} \\
 & - \frac{(8 - 13y^2 + 7y^3) H_{0,0,0,1,0}}{32(1-y)y} - \frac{(10 + 2y - 15y^2 + 6y^3) H_{0,0,1,0,0}}{32(1-y)y} \\
 & + \frac{(2 - 2y - y^2 + 2y^3) H_{0,0,1,1,0}}{32(1-y)y} - \frac{(12 - 19y + 13y^2 + 2y^3) H_{0,1,0,0,0}}{32(1-y)y} \\
 & - \frac{(6 - 7y + 3y^2 + y^3) H_{0,1,0,1,0}}{32(1-y)y} - \frac{(6 + 21y - 25y^2 - y^3) H_{0,1,1,0,0}}{32(1-y)y} + \frac{(6 + y) H_{2,1,1,1,0}}{16} \\
 & + \frac{(2 - 28y - 11y^2) H_{0,1,1,1,0}}{32y} - \frac{(15 + 13y - 12y^2 - 6y^3) H_{1,0,0,0,0}}{32(1-y)y} - \frac{(3 + 2y) H_{1,0,1,1,0}}{32} \\
 & - \frac{(4 + 16y - 26y^2 + 5y^3) H_{1,0,0,1,0}}{32(1-y)y} - \frac{(4 + 23y - 37y^2 + 7y^3) H_{1,0,1,0,0}}{32(1-y)y} \\
 & + \frac{(18 + 30y - 31y^2 - 5y^3) H_{1,1,0,0,0}}{64(1-y)y} - \frac{(2 + 10y - y^2) H_{1,1,0,1,0}}{32y} - \frac{(6 + y) H_{2,1,0,0,0}}{8} \\
 & - \frac{(2 + 5y - y^2) H_{1,1,1,0,0}}{8y} - \frac{(2 + 30y - y^2) H_{1,1,1,1,0}}{32y} + \frac{(6 + y) H_{2,1,1,0,0}}{16} \\
 & - \frac{(296 - 221y - 51y^2) \zeta_5}{128(1-y)} + \frac{(270 - 253y - 33y^2) \pi^2 \zeta_3}{384(1-y)} + \zeta_3 \left[\frac{P_{64}}{384(1-y)(2-y)^4 y} \right. \\
 & + \frac{H_0 P_{65}}{192(1-y)} - \frac{H_1 P_{66}}{192(1-y)(2-y)^5 y^2} - \frac{(2 - 6y + 5y^2) H_{0,0}}{16(1-y)} - \frac{(6 + y) H_{2,1}}{8} \\
 & \left. - \frac{(8 - 65y + 48y^2 + 14y^3) H_{0,1}}{32(1-y)y} - \frac{(2 - y)(2 + 4y - 5y^2) H_{1,0}}{32(1-y)y} + \frac{3(2 + 10y - y^2) H_{1,1}}{32y} \right] \\
 & + \pi^4 \left[-\frac{P_{67}}{138240(1-y)} - \frac{(192 - 293y + 106y^2) H_0}{11520(1-y)} + \frac{(104 + 375y - 58y^2) H_1}{11520y} \right] \\
 & + \pi^2 \left[\frac{P_{78}}{82944y(1-y)(2-y)^3} - \frac{P_{79} H_0}{4608y(1-y)} - \frac{P_{80} H_1}{13824y(1-y)(2-y)^4} \right. \\
 & + \frac{P_{81} H_{0,0}}{2304(1-y)^2} + \frac{P_{82} H_{0,1}}{2304y} - \frac{P_{83} H_{1,0}}{2304y^2(1-y)} + \frac{P_{84} H_{1,1}}{2304y^2(1-y)(2-y)^5} \\
 & - \frac{(24 - 25y + 9y^2) H_{0,0,0}}{192(1-y)} + \frac{(2 - 2y - y^2 + 2y^3) H_{0,0,1}}{192y(1-y)} - \frac{(2 - 31y - 9y^2) H_{0,1,0}}{192y} \\
 & + \frac{(2 - 28y - 11y^2) H_{0,1,1}}{192y} - \frac{(2 + 38y - 60y^2 + 13y^3) H_{1,0,0}}{192y(1-y)} - \frac{(3 + 2y) H_{1,0,1}}{192} \\
 & \left. + \frac{(14 + 50y - 11y^2) H_{1,1,0}}{384y} - \frac{(2 + 30y - y^2) H_{1,1,1}}{192y} + \frac{(6 + y) H_{2,1,1}}{96} \right] \Big\}. \tag{B.3}
 \end{aligned}$$

For convenience, we introduced the polynomials

$$\begin{aligned}
P_1 &= 32 - 24y - 23y^2 - 39y^3 + 22y^4 - 4y^5, \\
P_2 &= 8 - 32y + 45y^3 - 10y^4 - 11y^5 - 5y^6 - 2y^7 + y^8, \\
P_3 &= 6 - 27y + 14y^2 - 3y^3 + 2y^4 - y^5, \\
P_4 &= 8 - 32y + 8y^2 + 47y^3 - 46y^4 - 2y^5 + 8y^6, \\
P_5 &= 48 + 412y - 591y^2 + 128y^3 + 81y^4 - 6y^5, \\
P_6 &= 8 - 32y + 45y^3 - 10y^4 - 11y^5 - 5y^6 - 2y^7 + y^8, \\
P_7 &= 8 - 24y + 6y^2 + 44y^3 - 17y^4 - 2y^5, \\
P_8 &= 768 - 3264y + 4640y^2 + 610y^3 - 14070y^4 + 23584y^5 - 16792y^6 + 5265y^7 - 450y^8 \\
&\quad - 57y^9 + 9y^{10}, \\
P_9 &= 24 - 96y + 134y^2 + 114y^3 - 189y^4 + 76y^5, \\
P_{10} &= \sqrt{4-y}\sqrt{y}(232 + 306y - 1279y^2 + 1085y^3 - 297y^4 + y^5 + 6y^6), \\
P_{11} &= 8 - 36y + 60y^2 + 18y^3 - 84y^4 + 54y^5 - 11y^6, \\
P_{12} &= 32 - 126y + 186y^2 + 167y^3 - 381y^4 + 201y^5 - 19y^6 - 6y^7, \\
P_{13} &= 12288 - 47328y + 524580y^2 - 1178622y^3 + 970722y^4 - 316577y^5 + 49742y^6 \\
&\quad - 9103y^7 + 946y^8 - 48y^9, \\
P_{14} &= 576 - 713y + 1620y^2 - 2812y^3 + 783y^4 - 66y^5, \\
P_{15} &= \sqrt{4-y}\sqrt{y}(384 - 1408y + 1852y^2 - 1025y^3 + 265y^4 - 34y^5 + 2y^6), \\
P_{16} &= 64 - 144y - 48y^2 + 59y^3 - 13y^4 + 88y^5 - 104y^6 - 27y^7 + 13y^8, \\
P_{17} &= 160 - 484y + 301y^2 - 435y^3 + 62y^4 - 74y^5 + 26y^6, \\
P_{18} &= 128 - 256y - 74y^2 + 533y^3 - 444y^4 - 286y^5 + 395y^6 - 102y^7 + 4y^8, \\
P_{19} &= 192 - 108y - 1430y^2 + 2460y^3 - 1651y^4 + 602y^5 - 105y^6 + 4y^7, \\
P_{20} &= 8 - 24y - 4y^2 + 31y^3 + y^4 - 10y^5 + y^6 - y^7, \\
P_{21} &= 40 - 160y - 80y^2 + 265y^3 + 30y^4 - 55y^5 - 89y^6 - 10y^7 + 5y^8, \\
P_{22} &= 8 - 40y + 28y^2 + 23y^3 - 26y^4 + 41y^5 - 52y^6 + 24y^7, \\
P_{23} &= 22 + 105y + 43y^2 - 33y^3 - 31y^4 - 3y^5 + 3y^6, \\
P_{24} &= 16 - 80y + 82y^2 - 31y^3 + 39y^4 - 26y^5 + 13y^6 + y^7 - 3y^8 + y^9, \\
P_{25} &= 150 - 336y + 267y^2 - 86y^3 + 19y^4 - 2y^5, \\
P_{26} &= 40 - 160y - 35y^2 + 261y^3 - 246y^4 + 18y^5 + 34y^6 - 4y^7 + 2y^8, \\
P_{27} &= 40 - 160y + 320y^2 - 347y^3 + 104y^4 - 3y^5 + 8y^6 + 4y^7 - 2y^8, \\
P_{28} &= 38 - 136y + 209y^2 - 118y^3 + 17y^4 + 2y^5, \\
P_{29} &= 38 - 136y + 209y^2 - 118y^3 + 17y^4 + 2y^5, \\
P_{30} &= 69 - 320y + 223y^2 + 12y^3 + 8y^4 - 4y^5, \\
P_{31} &= 4608 - 448416y - 659436y^2 + 4185274y^3 - 4799654y^4 + 1822435y^5 - 149226y^6 \\
&\quad + 27309y^7 - 2838y^8 + 144y^9, \\
P_{32} &= 540 + 8440y - 7893y^2 + 284y^3 + 4011y^4 - 99y^5,
\end{aligned}$$

$$\begin{aligned}
P_{33} &= \sqrt{4-y}\sqrt{y}(384 - 1408y + 1852y^2 - 1025y^3 + 265y^4 - 34y^5 + 2y^6), \\
P_{34} &= 64 - 144y - 48y^2 + 59y^3 - 13y^4 + 88y^5 - 104y^6 - 27y^7 + 13y^8, \\
P_{35} &= 80 + 1348y - 1952y^2 + 1063y^3 + 7y^4 - 37y^5 + 13y^6, \\
P_{36} &= 384 - 984y + 1718y^2 + 749y^3 - 4359y^4 + 4207y^5 - 1163y^6 - 24y^7 + 12y^8, \\
P_{37} &= 192 - 108y - 1430y^2 + 2460y^3 - 1651y^4 + 602y^5 - 105y^6 + 4y^7, \\
P_{38} &= 8 - 24y - 4y^2 + 31y^3 + y^4 - 10y^5 + y^6 - y^7, \\
P_{39} &= 40 - 160y - 80y^2 + 265y^3 + 30y^4 - 55y^5 - 89y^6 - 10y^7 + 5y^8, \\
P_{40} &= 8 - 40y + 28y^2 + 23y^3 - 26y^4 + 41y^5 - 52y^6 + 24y^7, \\
P_{41} &= 736 - 161y - 634y^2 + 236y^3 - 141y^4 - 9y^5 + 9y^6, \\
P_{42} &= 32 - 160y + 409y^2 - 412y^3 - 3y^4 + 240y^5 - 104y^6 + 26y^7 - 6y^8 + 2y^9, \\
P_{43} &= 150 - 336y + 267y^2 - 86y^3 + 19y^4 - 2y^5, \\
P_{44} &= 40 - 120y + 155y^2 + 336y^3 - 139y^4 - 2y^5 + 2y^6 - 2y^7, \\
P_{45} &= 40 - 120y + 287y^2 - 52y^3 - 25y^4 - 4y^5 - 2y^6 + 2y^7, \\
P_{46} &= 38 - 136y + 209y^2 - 118y^3 + 17y^4 + 2y^5, \\
P_{47} &= 38 - 136y + 209y^2 - 118y^3 + 17y^4 + 2y^5, \\
P_{48} &= 60 - 227y + 199y^2 + 6y^3 + 8y^4 - 4y^5, \\
P_{49} &= 18144 - 717664y + 1393886y^2 - 1133657y^3 + 67075y^4 + 119280y^5, \\
P_{50} &= 274192 - 790576y + 1022744y^2 - 729184y^3 + 291089y^4 - 60673y^5 + 5656y^6 - 168y^7, \\
P_{51} &= 3024 - 61016y + 183708y^2 - 236394y^3 + 76836y^4 + 100086y^5 - 104001y^6 \\
&\quad + 36935y^7 - 5091y^8 + 126y^9, \\
P_{52} &= 272992 - 1044080y + 1562576y^2 - 1232952y^3 + 571342y^4 - 159511y^5 + 24578y^6 \\
&\quad - 1221y^7 - 126y^8, \\
P_{53} &= 6314 - 2172y - 4044y^2 + 2395y^3 - 1047y^4 - 42y^5, \\
P_{54} &= 97760 - 171536y + 8736y^2 + 228808y^3 - 283210y^4 + 175611y^5 - 62971y^6 + 12211y^7 \\
&\quad - 831y^8 - 42y^9, \\
P_{55} &= 32096 - 37872y - 79008y^2 + 208376y^3 - 194594y^4 + 92685y^5 - 23367y^6 + 3151y^7 \\
&\quad - 321y^8 + 42y^9, \\
P_{56} &= 1180 - 1728y + 726y^2 - 110y^3 + 7y^4 + 12y^5 - 7y^6, \\
P_{57} &= 256 - 12y - 350y^2 + 144y^3 + 4y^4 - 5y^5 + 7y^6, \\
P_{58} &= 210 - 40y - 230y^2 + 66y^3 + 4y^4 - 5y^5 + 7y^6, \\
P_{59} &= 218 + 102y - 78y^2 + 18y^3 - 2y^4 - 7y^5, \\
P_{60} &= 10368 - 5472y - 57616y^2 + 122720y^3 - 112960y^4 + 57278y^5 - 16673y^6 + 2248y^7 \\
&\quad + 375y^8 - 302y^9 + 75y^{10} - 7y^{11}, \\
P_{61} &= 104 + 233y - 303y^2 + 8y^3 - 4y^4 + 5y^5 - 7y^6, \\
P_{62} &= 13696 - 6208y - 70768y^2 + 138280y^3 - 113064y^4 + 47190y^5 - 10067y^6 + 1549y^7 \\
&\quad - 730y^8 + 334y^9 - 75y^{10} + 7y^{11},
\end{aligned}$$

$$\begin{aligned}
P_{63} &= 3520 - 26656y + 95616y^2 - 179744y^3 + 192708y^4 - 125322y^5 + 52036y^6 \\
&\quad - 14721y^7 + 2727y^8 + 66y^9 - 262y^{10} + 75y^{11} - 7y^{12}, \\
P_{64} &= 1760 - 10016y + 16128y^2 + 2464y^3 - 25794y^4 + 24018y^5 - 9947y^6 + 2078y^7 \\
&\quad - 219y^8 + 14y^9, \\
P_{65} &= 54 - 71y - 27y^2 + 8y^3 + 5y^4 - 7y^5, \\
P_{66} &= 1760 - 9808y + 45568y^2 - 105240y^3 + 126518y^4 - 85905y^5 + 34147y^6 - 7867y^7 \\
&\quad + 635y^8 + 476y^9 - 298y^{10} + 75y^{11} - 7y^{12}, \\
P_{67} &= 174 - 2916y + 6144y^2 - 2116y^3 - 25y^4 + 35y^5, \\
P_{68} &= 8 - 28y + 17y^2 + 5y^3 + 2y^4 - y^5, \\
P_{69} &= -31 + 31y + 30y^2 - 23y^3 - 2y^4 + y^5, \\
P_{70} &= 40 - 160y + 234y^2 - 113y^3 - 108y^4 + 49y^5 + 26y^6 + 4y^7 - 2y^8, \\
P_{71} &= 8 - 32y - 20y^2 + 55y^3 + 10y^4 - 11y^5 - 21y^6 - 2y^7 + y^8, \\
P_{72} &= 132 + 73y - 299y^2 - 43y^3 + 107y^4 + 3y^5 - 3y^6, \\
P_{73} &= 128 - 416y + 1406y^2 - 859y^3 - 1053y^4 + 522y^5 + 50y^6 - 26y^7, \\
P_{74} &= 192 - 624y + 88y^2 - 936y^3 + 1991y^4 - 273y^5 + 75y^6 - 39y^7, \\
P_{75} &= 136 - 75y - 20y^2 + 54y^3 - 47y^4 - 3y^5 + 3y^6, \\
P_{76} &= 40 - 160y + 321y^2 - 105y^3 - 185y^4 + 73y^5 + 20y^6 + 4y^7 - 2y^8, \\
P_{77} &= 8 - 32y - 20y^2 + 55y^3 + 10y^4 - 11y^5 - 21y^6 - 2y^7 + y^8, \\
P_{78} &= -25344 - 1042816y + 2510712y^2 - 1375772y^3 - 788722y^4 + 1105035y^5 \\
&\quad - 413921y^6 + 54480y^7 - 504y^8, \\
P_{79} &= -176 - 4132y + 6149y^2 - 848y^3 - 925y^4 - 14y^5, \\
P_{80} &= 32096 - 37872y - 79008y^2 + 208376y^3 - 194594y^4 + 92685y^5 - 23367y^6 \\
&\quad + 3151y^7 - 321y^8 + 42y^9, \\
P_{81} &= -732 + 3118y - 3086y^2 + 840y^3 - 39y^4 - 12y^5 + 7y^6, \\
P_{82} &= 218 + 102y - 78y^2 + 18y^3 - 2y^4 - 7y^5, \\
P_{83} &= 88 - 590y - 73y^2 + 760y^3 - 41y^4 - 92y^5 - 5y^6 + 7y^7, \\
P_{84} &= 3520 - 26656y + 95616y^2 - 179744y^3 + 192708y^4 - 125322y^5 + 52036y^6 \\
&\quad - 14721y^7 + 2727y^8 + 66y^9 - 262y^{10} + 75y^{11} - 7y^{12}.
\end{aligned} \tag{B.4}$$

Data Availability Statement. This article has data included as electronic supplementary material.

Code Availability Statement. This article has no associated code or the code will not be deposited.

Supplementary material and data. The following files are provided as supplementary material/data and are accessible through the article's webpage.

- esm.zip

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