Third order correction to semileptonic $b \to u$ decay: Fermionic contributions

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We present the QCD corrections of order α_s^3 to the decay rate of $b \to u\ell\bar{\nu}_\ell$, with $\ell = e, \mu$, originating from diagrams with closed fermion loops and neglecting the mass of the up quark. Our calculation relies on integration-by-parts reduction of Feynman integrals with one propagator raised to a symbolic power in KIRA and the numerical evaluation of master integrals with AMFlow. This allows us to obtain results for the fermionic contributions to the total semileptonic rate with an accuracy of more than 30 digits.

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I. INTRODUCTION

The inclusive B-meson decay $B \to X_u\ell\bar{\nu}_\ell$, with $\ell = e,\ \mu$, has a pivotal role in the extraction of the Cabbibo-Kobayashi-Maskawa matrix element $|V_{ub}|$ and in global fits of the unitarity triangle within the Standard Model [1,2].

Because of experimental cuts applied to semileptonic $b \to u$ decay to suppress the $b \to c$ contamination, the theoretical description of the differential rate for inclusive $B \to X_u\ell\bar{\nu}_\ell$ is based on a nonlocal operator product expansion (OPE) [3–5]. Perturbative coefficients in the OPE are convoluted with nonperturbative shape functions. Their exact form cannot be calculated from first principles so different parametrizations exist [6–10] which lead to $|V_{ub}|$ determinations with uncertainties of about 4% [11].

In this paper we consider the total $B \to X_u\ell\bar{\nu}_\ell$ decay rate which is cleaner from the theoretical point of view because it does not involve shape functions. The total rate is described by the heavy quark expansion [12–14], a local OPE in inverse powers of the bottom quark mass, which has been successfully applied to semileptonic $b \to c$ decays and the extraction of $|V_{cb}|$ [15,16].

The Belle II Collaboration [17] has recently presented a preliminary measurement of the ratio $\Gamma(B \to X_u\ell\bar{\nu}_\ell)/\Gamma(B \to X_c\ell\bar{\nu}_\ell)$ from which it is possible to extract $|V_{ub}/V_{cb}|$ given a prediction for the phase-space ratio [18–20]

$$C = \left|\frac{V_{ub}}{V_{cb}}\right|^2 \frac{\Gamma(B \to X_c\ell\bar{\nu}_\ell)}{\Gamma(B \to X_u\ell\bar{\nu}_\ell)}, \tag{1}$$

which is also employed to normalize the branching ratio of radiative decays ($B \to X_s\gamma$) and rare semileptonic decays ($B \to X_s\ell^+\ell^-$). The ratio C is determined using the heavy quark expansion together with measurements of the $B \to X_c\ell\bar{\nu}_\ell$ decay spectra. The current estimate $C = 0.568 \pm 0.007 \pm 0.010$ [21] has a 2.1% uncertainty that will be comparable with the future experimental error on $B \to X_s\gamma$, of about 2.6%, which is achievable with the full Belle II dataset [22]. Also for the theoretical prediction of the $B \to X_s\ell^+\ell^-$ branching fraction, the ratio C is a significant source of uncertainty [23–25].

In the free quark approximation the total rate of $b \to u\ell\bar{\nu}_\ell$ has been calculated up to $O(\alpha_s^2)$ in Refs. [26–28]. The third order correction has been estimated in Refs. [29,30] (see also Ref. [31]) by performing an asymptotic expansion for $\delta = 1 - m_c/m_b \to 0$, i.e. in the limit $m_b \simeq m_c$. The series in δ exhibits a fast convergence and allows us to obtain an accurate result for $b \to c$ decay at the physical value of the charm mass. Moreover, the expansion shows a good convergence even for $\delta \to 1$, corresponding to a massless final-state quark. This allows us to make an estimate of the charmless decay $b \to u$, however, with a 10% uncertainty on the α_s^3 correction due to the extrapolation to massless quark. This prediction has been recently confirmed by an independent calculation performed in the leading-color approximation [32] with an uncertainty of about 5% in the on-shell scheme, a factor of 2 improvement compared to Ref. [29]. This translates into a systematic 0.5% uncertainty on the total semileptonic rate.

In the present paper, we take a first step towards the improvement of the prediction for the total rate of $b \to u\ell\bar{\nu}_\ell$. We present the calculation of the fermionic contributions at order α_s^3, i.e., the subset of five-loop diagrams containing closed fermion loops. The evaluation

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of the remaining part, the bosonic corrections, is underway and it will be presented in a future publication. In Sec. II we describe the methods used for the calculation of five-loop diagrams, in particular, how we perform the integration-by-parts (IBP) reduction and the numerical evaluation of the master integrals. We present our results in Sec. III together with a comparison with previous calculations. We conclude in Sec. IV.

II. METHODS

We calculate higher order QCD corrections to the decay rate by employing the optical theorem and considering the imaginary part of self-energy diagrams like those shown in Fig. 1. At order α_s^3 we compute diagrams up to five loops. The Feynman diagrams contain a neutrino, a charged lepton, and an up quark as internal particles, which are all considered massless. Only the bottom quark is taken as massive and we normalize its mass to unity for simplicity. The Feynman integrals depend only on the dimensional regularization parameter $d = 4 - 2\epsilon$. The weak decay mediated by the W boson is treated with an effective four-fermion interaction, shown with black dots in Fig. 1.

In this paper we concentrate on the subset of gauge-invariant diagrams that contain at least one closed fermion loop, where the internal quark can be massless, u, d, s, c, or massive, the bottom quark [see for instance Figs. 1(a) and 1(b)]. We ignore the finite charm-mass effects.

For the computation of the bottom self-energy diagrams we use QGRAF [33] to generate the amplitude. We use the program TAPIR [34] for identification, manipulation, and minimization of Feynman integral families. With EXP [35,36] we generate a FORM [37–39] code to perform the Dirac and color algebra. We perform our calculation in Feynman gauge. We express the complete amplitude,

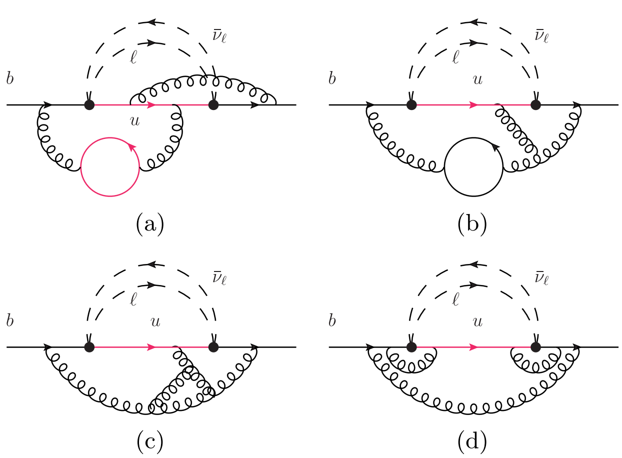

FIG. 1. Five-loop diagrams contributing to the α_s^3 correction to $b \to u\ell\bar{\nu}_\ell$. Sample of fermionic (a), (b) and bosonic (c), (d) contributions. Lepton and neutrino are shown with dashed lines; black and red solid lines represent the bottom and up quark. The effective vertex is shown by a dot.

fermionic, and bosonic contributions, as a linear combination of Feynman integrals belonging to 1, 21, and 107 integral families at three, four, and five loops, respectively.

We utilize IBP identities [40,41] and deploy Laporta's algorithm [42] to express all integrals appearing in the amplitude through a smaller set of integrals (for public tools see Refs. [43–47]). The reduction of the five-loop integrals constitutes the major bottleneck. The integral families at five loops contain up to 12 propagators and 8 irreducible numerators. Given that the amplitude needs an integral reduction in the top sector with up to 5 scalar products, this would generate a rich combinatorics when seeding the IBP vectors for the construction of IBP equations, leading to a huge RAM consumption of several TBs.

In order to perform the IBP reduction, we find it beneficial to integrate out the lepton-neutrino loop, which corresponds to a massless propagatorlike one-loop integral of the form

$$\int d^d p \frac{p^{\mu_1} \dots p^{\mu_N}}{(-p^2)[-(p-q)^2]} = \frac{i\pi^{2-\epsilon}}{(-q^2)^\epsilon} \sum_{i=0}^{[N/2]} f(\epsilon, i, N) \left(\frac{q^2}{2}\right)^i \{[g]^i [q]^{N-2i}\}^{\mu_1 \dots \mu_N}, \quad (2)$$

where the function $f(\epsilon, i, N)$ is a product of Euler's gamma functions (see, e.g., [48]) and the symbol $\{[g]^i[q]^{N-2i}\}^{\mu_1\dots\mu_N}$ stands for the tensor composed of i metric tensors and $N - 2i$ vectors q, which is totally symmetric in its indices. We rewrite the original five-loop topologies into four-loop ones that have a reduced number of propagator power indices, 14 instead of 20, where one propagator is now raised to a symbolic power a_0.

We work with the IBP reduction program KIRA [49,50] together with the finite field reconstruction library FireFly [51,52]. In particular, KIRA supports reductions with symbolic powers. First, we perform a reduction of seed integrals with at most two dots and one scalar product. After identifying the nontrivial sectors in each family, we study which sectors contain integrals with a physical cut and therefore an imaginary part [see for instance Fig. 2(a)]. Sectors whose integrals are only real valued [see the example in Fig. 2(b)] are neglected during the IBP reduction. We observe that for some families with several massive propagators, such sector selection allows us to eliminate up to 70% of the nontrivial sectors.

After this step, we proceed with the IBP reduction of the complete set of integrals appearing in the amplitude. We replace the symbolic power a_0 with $(4 - d)/2 = \epsilon$ in the IBP equations in order to have only one reduction variable instead of two. Moreover, we take the IBP vectors and eliminate redundant shift operators; in particular, we eliminate most of the operators which would shift the symbolic power. When seeding the IBP identities, it is

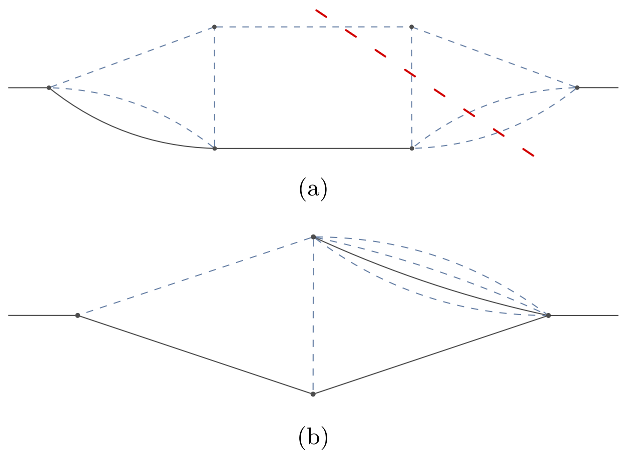

FIG. 2. Example of five-loop Feynman integrals. Black and dashed lines represent massive and massless propagators, respectively. Integral (a) has an imaginary part and we retain its sector during IBP reduction. Integral (b) has no physical cut so integrals belonging to the same sector can be discarded.

sufficient to have only zero or negative shifts of the symbolic power to reduce all necessary integrals.

The list of trivial sectors and symmetries derived for the five-loop topologies are translated to the four-loop ones. The four-loop master integrals are chosen such that no shift of the symbolic propagator power is allowed. The translation of four-loop master integrals back to five-loop master integrals is then trivial using Eq. (2) in the reverse direction.

For the fermionic contributions, the amplitude is reduced to 1369 master integrals with KIRA, which have, in the worst case, one scalar product belonging to 48 different integral families. The complete amplitude is reduced to 8845 master integrals which have up to two scalar products belonging to 107 integral families. Our setup is cross-checked with FIRE for ten integral families, where we perform the reduction over a prime field and a fixed value of d with FIRE6 [45].

To calculate the master integrals, we leverage the method of solving differential equations numerically (see, e.g., Refs. [53–57]). In this paper, we follow the strategy outlined in [58] and the auxiliary mass flow method, [54,59] which is implemented in the AMFlow package [60,61]. For similar approaches see also Refs. [62–71]. We calculate the five-loop master integrals numerically requiring 40 digits of precision using subroutines provided in AMFlow. We do not minimize the number of master integrals across different integral families because it is not crucial for the reduction of the overall runtime for the whole calculation.

The auxiliary mass flow method requires us to construct systems of differential equations with respect to the auxiliary mass η which is introduced into certain propagators. We implement in the framework of AMFlow our own interface to KIRA in order to perform the IBP reduction with the mapping from five-loop to four-loop topologies as described above. However, at this stage of the calculation one needs to consider all nontrivial sectors, not only those which generate an imaginary part. The IBP reductions to master integrals are more involved compared to the amplitude reduction since the additional scale η increases the number of master integrals.

III. RESULTS AND DISCUSSION

After the evaluation of the master integrals, we insert their results into the amplitude and perform the wave function and bottom mass renormalization in the on-shell scheme [72–75], while we use $\overline{\mathrm{MS}}$ for the strong coupling constant. The total rate for $b \to u$ decay can be written as

$$\Gamma(B \to X_u \ell \bar{\nu}_\ell) = \Gamma_0 \left[1 + C_F \sum_{n\geq 1} \left(\frac{\alpha_s}{\pi}\right)^n X_n\right] + O\left(\frac{\Lambda^2_{\mathrm{QCD}}}{m_b^2}\right), \tag{3}$$

where $\Gamma_0 = G_F^2 m_b^5 |V_{ub}|^2 A_{\mathrm{ew}}/(192\pi^3)$, $C_F = 4/3$, and $\alpha_s \equiv \alpha_s^{(5)}(\mu_s)$ is the coupling constant at the renormalization scale μ_s. $A_{\mathrm{ew}} = 1.014$ is the leading electroweak correction, [76] and m_b is the on-shell mass of the bottom quark. The coefficient X_3 at order α_s^3 can be divided into 10 color structures:

$$\begin{aligned} X_3 = {} & N_L^2 T_F^2 X_{N_L^2} + N_H^2 T_F^2 X_{N_H^2} + N_H N_L T_F^2 X_{N_H N_L} \\ & + N_L T_F (C_F X_{N_L C_F} + C_A X_{N_L C_A}) \\ & + N_H T_F (C_F X_{N_H C_F} + C_A X_{N_H C_A}) \\ & + C_F^2 X_{C_F^2} + C_F C_A X_{C_F C_A} + C_A^2 X_{C_A^2}, \end{aligned} \tag{4}$$

with $C_F = (N_c^2 - 1)/(2N_c)$, $C_A = N_c$, and $T_F = 1/2$ for an $SU(N_c)$ gauge group. Here $N_L = 4$ is the number of massless quarks and $N_H = 1$ labels the b-quark loop. The first seven color structures are the fermionic contributions while the last three stem from diagrams where only gluons are exchanged.

We estimate the precision of our result from the numerical pole cancellations of the renormalized decay rate. We have analytic expressions for the bare amplitude up to order α_s, while at $O(\alpha_s^2)$ the amplitude is obtained via numerical evaluation of the master integrals with 80 digits of precision. We observe that in X_3 the ϵ^{-3}, ϵ^{-2}, and ϵ^{-1} poles cancel with more than 37, 35, and 33 digits, respectively. Extrapolating those numbers to the finite terms, we expect that our results are correct up to 30 digits.

We present in Table I compact results for the first seven color factors at the renormalization scale $\mu_s = m_b$, reporting in the second column the first five significant digits. In the third column, we compare our results with Ref. [29] where we use the asymptotic expansion up to δ^{12} for the central value and estimate the uncertainty from the difference between the δ^{11} and δ^{12} expansion, multiplied by a security factor of five. We observe overall a good agreement within the uncertainties, except for the color structure $X_{N_L C_F}$ where

TABLE I. The first five digits of the color structure coefficients of X_3 in Eq. (4) at a renormalization scale $\mu_s = m_b$. The third and fourth column report the value from Ref. [29] and the relative difference, respectively.

	This work	Ref. [29]	Difference [%]
$T_F^2 N_L^2$	-6.9195	$-6.34\ (42)$	8.3
$T_F^2 N_H^2$	-1.8768×10^{-2}	$-1.97(42) \times 10^{-2}$	5.0
$T_F^2 N_H N_L$	-1.2881×10^{-2}	$-1.1(1.1) \times 10^{-2}$	12
$C_F T_F N_L$	-7.1876	$-5.65(55)$	22
$C_A T_F N_L$	42.717	39.7(2.1)	7
$C_F T_F N_H$	2.1098	2.056(64)	2.5
$C_A T_F N_H$	-0.45059	$-0.449(18)$	0.4

the deviation is larger than the uncertainty based on the asymptotic series convergence.

As a cross-check, we compare our finding with Ref. [32] which presents analytic expressions for the leading-color contributions to X_3. After taking the large-N_c limit, our results proportional to N_L^2 and N_L agree with Eq. (13) of Ref. [32] with more than 30 digits.

We also update the prediction for the third order correction in the on-shell scheme:

$$\Gamma(B \to X_u \ell \bar{\nu}_\ell) = \Gamma_0 \left[1 - 2.413 \frac{\alpha_s}{\pi} - 21.3 \left(\frac{\alpha_s}{\pi} \right)^2 - 267.8(2.7) \left(\frac{\alpha_s}{\pi} \right)^3 \right], \tag{5}$$

where $X_3 = -200.9 \pm 2.0$. The value at $O(\alpha_s^3)$ is obtained by summing our fermionic contributions and the analytic expression for the bosonic contribution in the large-N_c limit from Ref. [32]. Moreover, we add the subleading color terms which result from the calculation in Ref. [29]. The quoted uncertainty arises from the massless extrapolation and it is estimated as in Table I. The uncertainty is reduced by a factor of 4 compared to Ref. [32] and a factor of 10 with respect to Ref. [29].

IV. CONCLUSIONS

We presented the fermionic contributions to the decay rate of $b \to u \ell \bar{\nu}_\ell$ at order α_s^3. Our calculation is based on IBP reductions of Feynman integrals with a symbolic propagator power and numerical evaluation of master integrals via the auxiliary mass flow method. We estimate that our results have an accuracy of at least 30 digits.

The calculation of the missing three color structures coming from the bosonic contributions is ongoing. The method described in this paper can also be applied to the calculation of the finite charm-mass effects, although requiring additional computer resources due to the new scale m_c/m_b appearing in the Feynman integrals.

The decay rate $\Gamma(B \to X_u \ell \bar{\nu}_\ell)$ is an important ingredient in the normalization of radiative and rare semileptonic decays of B meson and can be employed to reduce the current theoretical uncertainty on the phase-space ratio C.

Note added. After the acceptance of our manuscript, the authors of Ref. [77] made available their unpublished results for the coefficients of N_L and N_L^2 in Eq. (4), which agree well with our results in the Table I.

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