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Taming the N3LO corrections to semileptonic $b \to u$ decay

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We review the calculation of the QCD corrections of order α_s^3 to the decay rate of $b \to u l \bar{\nu}_l$, originating from diagrams with closed fermion loops and neglecting the mass of the up quark. Our calculation takes advantage of integration-by-parts reduction of Feynman integrals with one propagator raised to a symbolic power in `Kira`. The five-loop master integrals are then evaluated numerically with the auxiliary mass flow method as implemented in `AMFlow`, in combination with an *ad hoc* interface to `Kira`. We obtain results for the fermionic contributions to the total semileptonic rate with an accuracy of more than thirty digits.

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1. Introduction

The decay $B \to X_s\gamma$ is a pivotal probe of new physics beyond the Standard Model (SM). Thus, it is essential to measure it with the highest accuracy and to provide precise predictions in the SM. The width of inclusive B decays has a strong sensitivity the value of m_b, the bottom quark mass, since it depends on the fifth power of m_b. In order to reduce the uncertainty on it, Gambino and Misiak proposed in [1] to express the rate of $B \to X_s\gamma$ in terms of the CKM favoured semileptonic $\mathrm{Br}(B \to X_c l\bar{\nu}_l)$. Normalising the rare B decay to the semileptonic width, i.e.

$$\mathrm{Br}(B \to X_s\gamma)_{E_\gamma > E_0} = \tau_B\,\Gamma(B \to X_c l\bar{\nu}_l)\,\frac{\Gamma(B \to X_s\gamma)_{E_\gamma > E_0}}{\Gamma(B \to X_c l\bar{\nu}_l)}, \quad (1)$$

is also advantageous because the ratio between $B \to X_s\gamma$ and $B \to X_c l\bar{\nu}_l$ depends on the CKM factor $\frac{|V_{ts}^\star V_{tb}|^2}{|V_{cb}|^2} \simeq \frac{[1+\lambda^2(2\bar{\rho}-1)+O(\lambda^4)]|V_{cb}|^2}{|V_{cb}|^2} = (0.965 \pm 0.001)$ known to permill level. In Eq. (1), the ratio on the r.h.s. is calculated within the heavy quark expansion (HQE) by making a double expansion in the strong coupling constant α_s and inverse power of m_b. However, the r.h.s. has a considerable dependence on the charm quark mass entering already at tree level in $\Gamma(B \to X_c l\bar{\nu}_l)$. For $B \to X_s\gamma$, the charm mass dependence arises at two loops from the interference between the four-quark operators (Q_1 and Q_2) and the electromagnetic dipole operator (Q_7) in the $\Delta B = \Delta S = 1$ effective Hamiltonian.

Therefore, to normalise the rate of $B \to X_s\gamma$ one can write instead

$$\mathrm{Br}(B \to X_s\gamma)_{E_\gamma > E_0} = \frac{\tau_B\,\Gamma(B \to X_c l\bar{\nu}_l)}{C}\,\frac{\Gamma(B \to X_s\gamma)_{E_\gamma > E_0}}{|V_{cb}|^2/|V_{ub}|^2\Gamma(B \to X_u l\bar{\nu}_l)} \quad (2)$$

where the phase-space ratio C is given by

$$C = \left|\frac{V_{ub}}{V_{cb}}\right|^2 \frac{\Gamma(B \to X_c l\bar{\nu}_l)}{\Gamma(B \to X_u l\bar{\nu}_l)}. \quad (3)$$

In Eq. (2) the width of $B \to X_s\gamma$ is normalized to the charmless semileptonic decay. The charm mass dependence is now clearly separated between the perturbative matrix elements of $b \to X_s\gamma$, which is a two-loop effect, and the normalization factor C which is a tree-level effect. The ratio C can be calculated using the HQE.

The most precise theory prediction for $B \to X_s\gamma$ from Refs. [2, 3] has an uncertainty of 5% and is given by

$$\mathcal{B}(B \to X_s\gamma)\Big|_{E_\gamma > 1.6\ \mathrm{GeV}} = (3.40 \pm 0.17) \times 10^{-4}, \quad (4)$$

where the updates from Ref. [4] are taken into account. The decay $B \to X_s\gamma$ is to leading order in the $1/m_b$ expansion given by the decay of a free quark $b \to X_s\gamma$. The prediction in Eq. (4) includes next-to-next-to-leading order (NNLO) QCD corrections. However, for charm mass dependence, only an interpolation from a large charm quark mass [5, 6] to a massless charm quark [3] is available, which is responsible for 3% of the uncertainty cited in Eq. (4). The remaining theoretical uncertainties are due to unknown higher-order corrections (3%) and other input in the heavy quark expansion (2.5%), like the quark masses and the non perturbative parameters.

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Recently, there has been significant progress towards completing the NNLO prediction for $B \to X_s\gamma$ with exact dependence on the charm mass [4, 7, 8]. For an update of the SM prediction for $B \to X_s\gamma$, it would therefore be desirable to determine the normalization factor C in Eq. (2) one order higher in α_s w.r.t. $\Gamma(B \to X_s\gamma)$, i.e. including corrections up to next-to-next-to-next-to-leading order (N3LO) at partonic level. The total rate of $B \to X_c l\bar{\nu}_l$ was calculated at N3LO in Refs. [9, 10] (see also Ref. [11]) by performing an asymptotic expansion for $\delta = 1 - m_c/m_b$ with $\delta \ll 1$, i.e. the limit of equally heavy b and c quarks $m_c \simeq m_b$. The expansion in δ exhibits a fast convergence and allows to obtain accurate results for $b \to c$ decay at the physical value of the charm mass.

In the free quark approximation the total rate of $b \to u\ell\bar{\nu}_\ell$ was calculated up to $O(\alpha_s^2)$ in Refs. [12–14]. The third order correction was also assessed in Refs. [9, 10] by noticing that the expansion in δ shows a good convergence even for the massless final-state quark, happening for $\delta \to 1$. The massless extrapolation allows to estimate $\Gamma(B \to X_u l\bar{\nu}_l)$ with a 10% uncertainty and results in a systematic 1% uncertainty on $\Gamma(B \to X_u l\bar{\nu}_l)$.

In Ref. [15] it has been observed furthermore that $\Gamma(B \to X_c l\bar{\nu}_l)$ obtained from the asymptotic expansion for $m_c \simeq m_b$ neglects subprocesses where there are three charm quarks in the final state like $b \to c\bar{c}cl\bar{\nu}_l$. Since this decay mode is allowed only for $m_c/m_b < 1/3$, the expansion for $m_c/m_b \simeq 1$ does not include three-charm contributions. Although the branching ratio for $b \to c\bar{c}cl\bar{\nu}_l$ is below 10^{-7} for physical values of the charm mass and thus negligible, it exhibits a logarithmic enhancement as $m_c \to 0$. Therefore, the validity of the extrapolation of to $\Gamma(B \to X_c l\bar{\nu}_l)$ computed in [9] to massless up quarks remains questionable.

All these considerations prompted a new calculation of the N3LO corrections to $B \to X_u l\bar{\nu}_l$ strictly with up quark mass set to zero. In the these proceeding, we review the calculation of fermionic contributions (the subset of five-loop diagrams containing closed fermion loops) to the total rate of $b \to u\ell\bar{\nu}_\ell$ at order α_s^3 presented in Ref. [16].

2. Technicalities

To extract the $O(\alpha_s^3)$ correction to the total rate, we compute the imaginary part of diagrams like those shown in Fig. 1 up to five loops. They contain a neutrino, a charged lepton and an up quark as internal particles, which are all considered massless. Only the bottom quark is massive and we set $m_b = 1$ for simplicity, so that Feynman integrals depend only on $\epsilon = (4 - d)/2$. The weak decay mediated by the W boson is treated with an effective four-quark operator. We provide results for the subset of gauge-invariant diagrams containing at least one closed fermion loop, with massless (u, d, s, c) or massive internal quarks [see e.g. Figs. 1(a) and 1(b)].

For our calculation we use a well-tested chain of programs which allows for a high degree of automation. We us `qgraf` [17] for the generation of the amplitude and `tapir` [18] for the translation to `FORM` [19] code and the identification of the underlying integral families. The program `exp` [20, 21] performs the mapping of the amplitudes to the integral families and prepares them for further processing with `FORM`. We express the complete amplitude, fermionic and bosonic contributions, as linear combination of Feynman integrals belonging to 1, 21 and 107 integral families at three, four and five loops, respectively.

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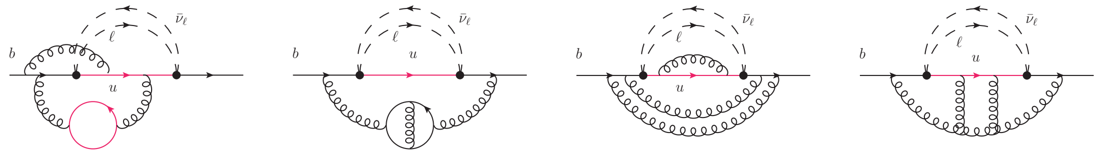

Figure 1: Five-loop diagrams contributing to the α_s^3 correction to $b \to u l \bar{\nu}_l$. Sample of fermionic (a,b) and bosonic (c,d) contributions. Lepton and neutrino are shown with dashed lines, black and red solid lines represent the bottom and up quark. The effective vertex is shown by a dot.

The IBP reduction of the integrals at five loops constitutes one of the major bottleneck in the calculation. We use the IBP reduction program `Kira` [22, 23] together with the finite field reconstruction library `FireFly` [24, 25]. At five loops the integral families contain up to 12 propagators and 8 irreducible numerators. Given that we need to reduce integrals in the top sector up rank five, i.e. sum of negative indices equal to five, one encounters a rich combinatorics when seeding the IBP vectors for the construction of IBP equations. In fact when seeding the lower subsectors, the program `Kira` considers all possible seed integrals with negative indices distributed in all possible ways across the non-positive indices. For subsectors with 10 to 15 non-positive indices, the list of seed candidates grows factorially and leads to a huge RAM memory consumption of several TBs when caching the IBP equations. In practice, with `Kira 2.3` we are not able to generate the system of IBP equations for the most complicated families.

In order to perform the IBP reduction, we reduce the number of loops by integrating out the lepton-neutrino loop analytically. Each family contains a massless propagator-like one-loop integral of the form

$$\int d^d p \frac{p^{\mu_1} \dots p^{\mu_N}}{(-p^2)[-(p-q)^2]} = \frac{i\pi^{2-\epsilon}}{(-q^2)^\epsilon} \times \sum_{i=0}^{[N/2]} f(\epsilon, i, N) \left(\frac{q^2}{2}\right)^i \{[g]^i [q]^{N-2i}\}^{\mu_1 \dots \mu_N}, \quad (5)$$

where the function $f(\epsilon, i, N)$ is product of Euler's gamma functions (see e.g. [26]) 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, totally symmetric in its indices. We rewrite the original five-loop topologies into four-loop ones that have a reduced number of indices: 14 instead of 20. Let us consider as an example the three-loop integral family

$$I(n_1, \dots, n_{)} =$$
$$\int \frac{d^d p_l}{(2\pi)^d} \frac{d^d q}{(2\pi)^d} \frac{d^d k}{(2\pi)^d} \frac{[(2p_l+q)^2]^{-n_6} [(k+p_l)^2]^{-n_7} [(k+p_l+q)^2]^{-n_8} [(p+p_l+q)^2]^{-n_9}}{[p_l^2]^{n_1} [(p_l+q)^2]^{n_2} [k^2]^{n_3} [(k-p+q)^2]^{n_4} [(p-q)^2]^{n_5}}, \quad (6)$$

where p is the momentum of the external bottom quark with the on-shell condition $p^2 = 1$. Using Eq. (5) we can map each integral in the family I with 9 indices onto a linear combination of elements of the family

$$J(n_1, \dots, n_5) = \int \frac{d^d q}{(2\pi)^d} \frac{d^d k}{(2\pi)^d} \frac{[(k+q)^2]^{-n_5}}{[-q^2]^{n_1} [k^2]^{n_2} [(k-p+q)^2]^{n_3} [(p-q)^2]^{n_4}} \quad (7)$$

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with only 5 indices. For instance

$$I(1,1,1,1,1,0,0,0,-1) = \frac{\Gamma^2(1-\epsilon)\Gamma(\epsilon)}{2\Gamma(2-2\epsilon)}\Big[J(\epsilon-1,1,1,1,0) - J(\epsilon,1,1,0,0) + 3J(\epsilon,1,1,1,0)\Big]. \tag{8}$$

However the new integrals present a propagator raised to a symbolic power $a_0 = \epsilon$. `Kira` supports reductions with symbolic powers via the option `symbolic_ibp: [...]`. The configuration file `integralfamilies.yaml` for family J would take the following form

```
integralfamilies:
  - name: "J"
    loop_momenta: [k,q]
    top_level_sectors: [15]
    propagators:
      - [ "q", 0]
      - [ "k", 0]
      - [ "k + q - p", 0]
      - [ "q - k", 0]
      - [ "k + q", 0]
    symbolic_ibp: [1]
```

where the last line tells `Kira` that the first propagator is raised to the power $n_1 + a_0$, where n_1 is an integer and a_0 an auxiliary symbol. In our case we can replace $a_0 = \epsilon$ to avoid performing the IBP reduction with two variables.

An additional speed up of the IBP reduction is given by the identification of the subsectors containing integrals without an imaginary part. Even if integrals in the top sector have by construction an imaginary part, integrals belonging some of the subsectors can be real-valued since cut propagators can get pinched (see the example in Fig. 2). To identify the sectors to retain during the IBP reduction, we perform for each family a first reduction of seed integrals with at most two dots and one scalar product. After identifying the nontrivial sectors, we study which sectors contain integrals with a physical cut. Sectors whose integrals are real valued (see the examples on the r.h.s. in Fig. 2) are excluded in `Kira` with the option `zero_sectors: [...]`. We observe that for families with several massive propagators, the sector selection allows to discard up to 70% of the nontrivial sectors, thus reducing the size of the IBP equation system.

By combining the two strategies aforementioned, we manage to perform the IBP reduction for all integrals in the amplitude. We select master integrals in the four loop families so that no shift of the symbolic propagator power is allowed. In this way we can convert the four-loop master integrals back to five-loop master integrals with the help of Eq. (5).

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` [27].

To calculate the master integrals, we use the auxiliary mass flow method [28, 29] and its implementation in the package `AMFlow` [30, 31]. The auxiliary mass flow method requires to

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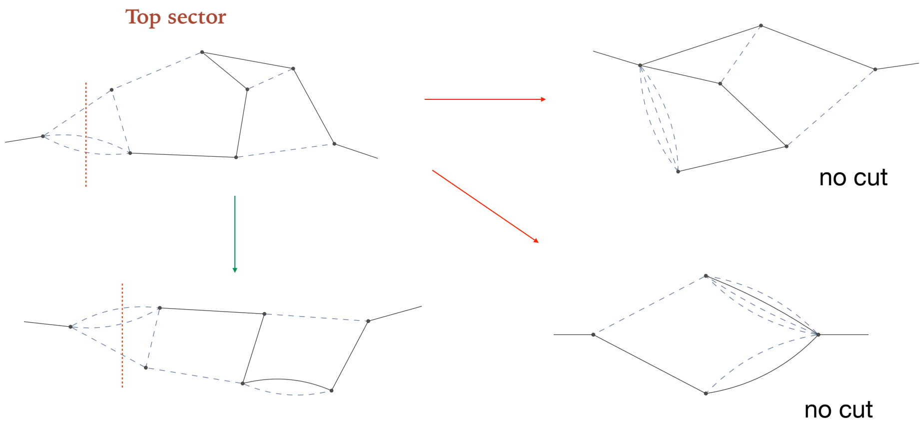

Figure 2: Example of five-loop Feynman integrals. Black and dashed lines represent massive and massless propagators, respectively. The integral on the top left side belong to the top sector of the family and has a physical cut (shown by the red dashed line). The integral on the bottom left belong to a subsector and has also an imaginary part, so we retain its sector in the IBP reduction. The integrals shown on the top and bottom right have no physical cut so their sectors can be discarded.

construct systems of differential equations with respect to the auxiliary mass η which is introduced into certain propagators. Even if the rank of the integrals to reduce is lower that the rank of the integrals in the amplitude, the presence of the additional variable η in the IBP reduction makes the calculation of the differential equations difficult. In the end, we observe that 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.

To simplify the problem, we implement in the framework of `AMFlow` our own interface to `Kira`. With our interface we are able to map the five-loop families with the mass parameter η to four-loop topologies using Eq. (5), avoiding to introduce η either in the electron or neutrino propagators. We then perform the IBP reduction with `Kira` and convert the result back to five-loop families when the IBP tables are returned to `AMFlow`. However at this stage, we need to consider all non-trivial sectors, not only those which generate an imaginary part.

With our setup, we calculate the five-loop master integrals by requiring 40 digits of precision, which is sufficient for phenomenological studies. We do not minimize the number of master integrals using symmetries among integral families. Such procedure would mainly map subsectors with fewer number of positive indices, leaving the top sectors of each family to large extend unmapped. The evaluation of these top-sector integrals with `AMFlow` would require in any case the evaluation of all master integrals belonging to the subsectors.

2.1 Results

We perform the renormalization of the bottom quark wave function and mass in the on-shell scheme [32–35], while we use $\overline{\text{MS}}$ renormalization for the strong coupling constant. The total rate for $b \to u$ is given by

$$\Gamma(B \to X_u \ell \bar{\nu}_\ell) = \Gamma_0 \left[1 + C_F \sum_{n \geq 1} \left(\frac{\alpha_s}{\pi} \right)^n X_n \right] + O\left(\frac{\Lambda_{\text{QCD}}^2}{m_b^2} \right), \tag{9}$$

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where $\Gamma_0 = G_F^2 m_b^5 |V_{ub}|^2 A_{\rm ew}/(192\pi^3)$, $C_F = 4/3$ and $\alpha_s \equiv \alpha_s^{(5)}(\mu_s)$ is the coupling constant at the renormalization scale μ_s. $A_{\rm ew} = 1.014$ is the leading electroweak correction [36] and m_b is the on-shell mass of the bottom quark. At the renormalization scale $\mu_s = m_b$, the coefficient at NLO [37] and NNLO [12] are

$$\begin{aligned}
X_1 =& \frac{25}{8} - \frac{\pi^2}{2}, \\
X_2 =& C_A \left(\frac{154927}{10368} + \frac{95\pi^2}{162} - \frac{53}{12}\pi^2 \log(2) - \frac{383\zeta_3}{72} + \frac{101\pi^4}{1440} \right) \\
&+ C_F \left(\frac{11047}{2592} - \frac{515\pi^2}{81} + \frac{53}{6}\pi^2 \log(2) - \frac{223\zeta_3}{36} + \frac{67\pi^4}{720} \right) \\
&+ N_H T_F \left(\frac{16987}{576} - \frac{85\pi^2}{216} - \frac{64\zeta_3}{3} \right) + N_L T_F \left(-\frac{1009}{288} + \frac{77\pi^2}{216} + \frac{8\zeta_3}{3} \right).
\end{aligned} \tag{10}$$

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. We approximate the charm quark as massless. Finite charm quark effects were calculated up to NNLO in [13, 14]. At order α_s^3 we obtain:

$$\begin{aligned}
X_3 =& - 0.0187678890858673847787492121610\, N_H^2 T_F^2 \\
&- 0.0128811414824744955979824846025\, N_H N_L T_F^2 \\
&- 6.91945963545141155160896317435\, N_L^2 T_F^2 \\
&+ (-0.450594547415538324373558306826\, C_A \\
&\quad + 2.10979928071936375821873123780\, C_F) N_H T_F \\
&+ (42.7167190901372543556242161718\, C_A \\
&\quad - 7.18755112505407688969676630368\, C_F) N_L T_F \\
&+ C_A^2 X_{C_A^2} + C_F^2 X_{C_F^2} + C_A C_F X_{C_F C_A}.
\end{aligned} \tag{11}$$

where we provide results for the color factors of the fermionic contributions up to 30 digits. 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 $\epsilon^{-3}, \epsilon^{-2}$ 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. The calculation of the last three color structures in Eq. (11) coming from the bosonic contributions will be presented in a future publication.

Our updated prediction for $b \to u l \bar{\nu}_l$ decay in the on-shell scheme to leading order in $1/m_b$ is

$$\Gamma(B \to X_u \ell \bar{\nu}_\ell) = \Gamma_0 \left[1 - 2.413 \frac{\alpha_s}{\pi} - 21.3 \left(\frac{\alpha_s}{\pi} \right)^2 - 267.8\,(2.7) \left(\frac{\alpha_s}{\pi} \right)^3 \right], \tag{12}$$

with $X_3 = -200.9 \pm 2.0$. 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. [38]. For the subleading colour terms of the bosonic contribution, we use the results from Ref. [9]. The quoted

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uncertainty arises from the massless extrapolation and it is estimated by taking the difference between the δ^{11} and δ^{12} expansions, multiplied by a security factor of five. The uncertainty is reduced by a factor of four compared to Ref. [38] and a factor of ten with respect to Ref. [9].

In the end, it is remarkable how close our prediction is compared to Ref. [9], $X_3^{[9]} = -202 \pm 20$, even in light of the fact that the $b \to c\bar{c}cl\bar{\nu}_l$ contribution is not accounted for while performing the asymptotic expansion in the limit $m_c \simeq m_b$ [15]. The prediction in Eq. (12) confirms the independent calculation performed in the leading-color approximation [38] which has an uncertainty of about 5% in the on-shell scheme. Moreover, the results for the fermionic color structures N_L^2 and N_L agree with the unpublished results for $b \to ul\bar{\nu}_l$ of Ref. [39].

3. Conclusions

In these proceedings we reviewed the calculation of the N3LO corrections to the total semileptonic width of $B \to X_u l\bar{\nu}_l$ to leading order in the heavy quark expansion. 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. Our numerical results have an accuracy of at least thirty digits, based on the $1/\epsilon$ pole cancellation happening at $O(\alpha_s^3)$.

The calculation of the missing three color structures coming from the bosonic contributions is ongoing. The major bottleneck here lies in the IBP reduction of certain integrals families with the auxiliary mass η inserted in some of the denominators. For these families, the generation of the system of differential equations in `AMFlow` is currently not competitive with `Kira-2.3`.

Since our publication [16], several bottlenecks have been eliminated in `Kira` and an improved integral seeding is currently being implemented [40]. With these improvements, we are able to generate, for the most complicated families in the bosonic sector, systems of differential equations with about a factor 10 reduction in the number of equations. With smaller systems, the time spent by `FireFly` is also reduced by more than a factor of 30 therefore making possible the calculation of the three missing color factors.

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