An Application of Rubi: Series Expansion of the Quark Mass Renormalization Group Equation

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Abstract

We highlight how Rule-based Integration (Rubi) is an enhanced method of symbolic integration which allows for the integration of many difficult integrals not accomplished by other computer algebra systems. Using Rubi, many simple techniques (e.g. linearly separable differential equations) become tractable. Integrals are step-wise simplified thus highlighting any unknown integration rules in difficult integrals. The motivating example we use is the derivation of the updated series expansion of the quark mass renormalization group equation (RGE) to fifth-loop order. This series provides the relation between a light quark mass in the modified minimal subtraction ($\overline{\text{MS}}$) scheme defined at some given scale, e.g. at the tau-lepton mass scale, and another chosen scale, μ. This relation explicitly depicts the renormalization scheme dependence of the running quark mass on the scale parameter, μ, and is important in accurately determining a light quark mass at a chosen scale. The latest coefficients of the QCD β and γ functions, β_4 and γ_4 respectively, are used in this determination.

Keywords: Rule-based integration (RUBI), Running quark mass, Quantum chromodynamics

1. Extensions to CAS by Rubi

Computer Algebra Systems (CAS) such as Mathematica (Wolfram Research, Inc., 2018) and SymPy (Meurer et al., 2017) (the popular open-source alternative implemented in Python), have built-in symbolic integral routines. Rule-based Integration (Rubi) developed by Rich (2018) is principally a package (designed for Mathematica) that provides a method of symbolic integration organized by decision tree pattern matching, which matches the form of the integral against known integral rules. Rubi comprises 6700+ rules, collated from familiar favourites Abramowitz and Stegun (1964); Beyer (1991); GradÅtejn and RyÅik (1994) and in doing so it offers not only a means of integrating, but a growing complete reference for integration rules. These rules are in human-readable form with cross references not only to Rubi rule numbers, but also to the source. Rubi can also print the rules applied at each stage of solving the integral – a useful technique not only for pedagogical purposes, but also diagnostically.

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Without proper consideration it may not be obvious why Rubi marks a significant improvement to effectively solving integrals. The effectiveness of these routines have been independently investigated by Abbasi (2018) with the results presented in Table 1. Comparing Rubi 4.15.2, Mathematica 11.3 and SymPy 1.1.1 Abbasi (2018) divides the quality of integral's antiderivatives into four groups. *Group A* consists of integrals that were easily solved: where the antiderivative is optimal in quality and leafsize. *Group B* is the group of integrals which were solved, but the leafsize twice that of optimal. *Group C's* integrals were solved, but the solution contains hypergeometric functions, special functions or imaginary units while the optimal antiderivative does not. Finally *Group F* are all integrals which cannot be solved by the CAS. See Abbasi (2018) for more details.

Table 1: Antiderivative Grade distribution for each CAS

System	% A grade	% B grade	% C grade	% F grade
Rubi	99.76	0.08	0.06	0.1
Mathematica	75.37	8.46	15.81	2.67
SymPy	30.29	0	0	69.71

Adapted: Abbasi (2018) pg. 5

Rule-based integration is the focus of much attention in development not only by Rich (2018), but by others. SymPy 1.1.1 currently fairs comparatively poorly in symbolic integration to other CAS (Table 1). However, the rules and implementation (pattern matching in a decision tree) behind Rubi are currently being developed into SymPy see Collaborators (2017) for details. This would clearly improve the quality of this open source alternative.

2. Motivating Example: the Quark Mass Renormalization Group Equation

Having examined how powerful Rubi is as a symbolic integration tool, we now explore how it can be applied in computation, using the quark mass renormalization group equation as a motivating example. Along with the strong coupling, the quark masses are fundamental parameters of Quantum Chromodynamics and it is therefore important to accurately know their numerical values. Further, it is important to know how scale dependent these values are.

In QCD, as in Quantum Electrodynamics (QED), one removes the present divergences with a technique known as renormalization. An energy scale, s, is introduced in the renormalization procedure to represent the point at which one performs the subtraction. Both the strong coupling $\alpha_s(s)$, and the quark masses, $m_q(s)$, depend on the renormalization scheme used to define the theory, and hence on the energy scale, s, which encodes the momentum dependence ($s = -q^2$). The s-dependence of $\alpha_s(s)$ and $\overline{m}_q(s)$ is governed by corresponding renormalization group equations (RGE's).

The strong coupling, $\alpha_s(s)$, satisfies the differential RGE (Davier et al., 2006):

$$\frac{da_s}{d\ln s} = \beta(a_s) = -a_s^2\,(\beta_0 + a_s\beta_1 + a_s^2\beta_2 + a_s^3\beta_3 + a_s^4\beta_4) \tag{1}$$

where the $\beta(a_s)$ function is known up to $O(a_s^6)$, and $a_s \equiv \frac{\alpha_s}{\pi} = \frac{g_s^2}{4\pi^2}$ (g_s is the gauge coupling of QCD).

While the quark masses, $m_q(s)$, satisfy the differential RGE (Davier et al., 2006):

$$\frac{1}{\overline{m}_q}\frac{d\overline{m}_q}{d\ln s} = \gamma(a_s) = -a_s\,(\gamma_0 \,+\, a_s\,\gamma_1 \,+\, a_s^2\,\gamma_2 \,+\, +a_s^3\,\gamma_3 \,+\, a_s^4\,\gamma_4) \tag{2}$$

where the $\gamma(a_s)$ function is known up to $O(a_s^5)$. The s-dependence of a_s and $\overline{m}_q$ of Eqs.(1)-(2) is implicit i.e. $a_s = a_s(s)$ and $\overline{m}_q = \overline{m}_q(s)$.

In the light quark sector (for three active quark flavours), the coefficients of the $\beta(a_s)$ function, which are now known to forth-loop order (Baikov et al., 2017), are given by: $\beta_0 = 9/4, \beta_1 = 4$, etc. While the $\gamma(a_s)$ function coefficients (also currently known to fourth-loop order (Baikov et al., 2014)) are: $\gamma_0 = 1$, $\gamma_1 = 91/24$, etc., for three flavours.

We concentrate on deriving the series expansion of Eq.(2) for the light quark sector, i.e. our result will be applicable for the up, down and strange quark. As we proceed to higher energies, i.e. into the heavy quark region, we cross certain flavour thresholds which will alter the numerical form of the perturbative expansion.

The recent calculation of the β_4 coefficient by Baikov et al. (2017), has ensured that the series expansion of the running quark mass can now be calculated to fifth-loop order. Previously this series expansion has been calculated by Chetyrkin et al. (1997) to fourth-loop order, which built on the third-loop order calculation done by Kniehl (1996). The perturbative series solution to Eq.(2) involves performing a taylor expansion of $\overline{m}_q(s)$ at some reference scale $s = s^*$, in powers of $\eta = \ln(s/s^*)$. To the third- and fourth-loop this calculation is a fairly trivial exercise. At higher loop orders, however, this computation becomes more difficult and CAS such as Mathematica and SymPy fail without the additional use of Rubi. We outline the method for using Rubi to find a perturbative solution to Eq.(2) in the following section. The derivation is purely symbolic.

3. The Perturbative Series Expansion of $\overline{m}_q(s)$

The quark mass RGE Eq.(2), can be identified as a linearly separable differential equation. As such, we are able to exactly for $\overline{m}_q$ given the coefficients of the $\beta(a_s)$ and $\gamma(a_s)$ functions to a certain order. The exact solutions to leading and next-to-leading order are given in Kniehl (1996). These solutions do not, however, provide insight into the renormalization scheme dependence of the running quark mass on the energy scale parameter, s, which is important in accurately determining the light quark mass at a chosen scale. It must also be remarked that it is difficult to obtain the exact solution of $\overline{m}_q$ at higher orders, and that this becomes a numerical procedure. It is therefore more lucid to solve the renormalization group equations in terms of a power expansion. Hence, we proceed with determining a perturbative series expansion of Eq.(2).

This is achieved by starting dividing Eq.(2) by Eq.(1) and linearly separating the differentials to yield

$$\frac{d\overline{m}_q}{\overline{m}_q} = \frac{\gamma(a_s)}{\beta(a_s)}\,da_s \tag{3}$$

where $\gamma(a_s)$ and $\beta(a_s)$ were defined in Eqs.(1)-(2).

Integrating Eq.(3) leads to

$$\ln\left(\frac{\overline{m}_q(s)}{\overline{m}_q(s^*)}\right) = \int_{a_s(s^*)}^{a_s(s)} da_s'\,\frac{\gamma(a_s')}{\beta(a_s')} \tag{4}$$

Which can be easily rearranged to find

$$\overline{m}_q(s) = \overline{m}_q(s^*)\ \exp\left(\int_{a_s(s_0)}^{a_s(s)} da'_s\, \frac{\gamma(a'_s)}{\beta(a'_s)}\right) \tag{5}$$

where $\bar{m}_q(s^*)$ is the initial condition.

Both Mathematica and Rubi can be used in attempts to solve the integral in Eq.(5). In terms of the integral classification we introduced in Section 1, we can classify the integral in Eq.(5) as a *Group F* integral, which means that Rubi (and other CAS) are unable to solve the integral analytically. Mathematica immediately yields an answer in terms of a RootSum object which, once the series expansion is performed, does not equal the perturbative expansion to the third-loop (Kniehl, 1996) or fourth-loop order (Chetyrkin et al., 1997); while Rubi's attempt is a partial solution involving lower order integrals. The advantage Rubi offers here is in simplification and clarity in identifying the unevaluated sections of the problem. This allows the researcher to focus on what Rubi does *not* know: rather than developing rules to solve integrals that Rubi already can solve, being aware of integrals that it cannot is useful for knowledge furthering. These integrals can then be suitably approximated.

Rubi's attempt at the indefinite version of the integral in Eq.(5) yields

$$\begin{aligned}
F(a'_s) \;&=\; \int da'_s\, \frac{\gamma(a'_s)}{\beta(a'_s)} \\
&=\; \frac{\gamma_0 \ln(a'_s)}{\beta_0} - \frac{1}{4\beta_0\beta_4}\Big\{(\beta_4\gamma_0 - \beta_0\gamma_4)\ \ln\left(\beta_0 + \beta_1 a'_s + \beta_2 {a'_s}^2 + \beta_3 {a'_s}^3 + \beta_4 {a'_s}^4\right) \\
&\quad +\ I_0\,(3\beta_1\beta_4\gamma_0 - 4\beta_0\beta_4\gamma_1 + \beta_0\beta_1\gamma_4)\ +\ 2\,I_1\,(\beta_2\beta_4\gamma_0 - 2\beta_0\beta_4\gamma_2 + \beta_0\beta_2\gamma_4) \\
&\quad + I_2\,(\beta_3\beta_4\gamma_0 - 4\beta_0\beta_4\gamma_3 + 3\beta_0\beta_3\gamma_4)\Big\}
\end{aligned} \tag{6}$$

where

$$I_n = \int da'_s\, \frac{{a'_s}^n}{\beta_0\ +\ \beta_1 a'_s\ +\ \beta_2 {a'_s}^2\ +\ \beta_3 {a'_s}^3\ +\ \beta_4 {a'_s}^4} \tag{7}$$

The integrals I_n, do not have an analytic solution in terms of algebraic functions and they can not be solved by Rubi unless certain assumptions are made. At this stage, Mathematica is able to re-write these integrals in terms of RootSum objects that can be suitably simplified when the series expansion is performed.

The definite integral of Eq.(6) is found simply by using the Fundamental Theorem of Calculus[1]. The upper bound of the definite integral, the scale dependent strong coupling $a_s(s)$, has a perturbative solution in terms of some known $a_s(s^*)$ (e.g. at the tau-lepton mass scale) up to $O(a_s^6)$ which is used here (Davier et al., 2006). The result is quite lengthy, despite some simplification occurring between polynomial sums arising from the I_n integrals in Eq.(6). It can be viewed in the supplementary Mathematica notebook.

Finally focusing on Eq.(5), we exponentiate the definite integral, and perform a series expansion at some reference scale $s = s^*$.

[1] An assumption of the Fundamental Theorem of Calculus is that the function to be integrated must be continuous. In the present case, the integrand is a rational function and therefore continuous up to isolated poles in the complex plane.

Reordering the perturbative solution in terms of $a_s(s^*)$ yields

$$\begin{aligned}
\overline{m}_q(s) \;=\; \overline{m}_q(s^*)\Big\{ & 1 - a(s^*)\,\gamma_0\,\eta + \frac{1}{2}\,a^2(s^*)\,\eta\Big[-2\,\gamma_1 + \gamma_0\,(\beta_0 + \gamma_0)\,\eta\Big] \\
& - \frac{1}{6}\,a^3(s^*)\,\eta\Big[6\,\gamma_2 - 3\Big(\beta_1\,\gamma_0 + 2\,(\beta_0 + \gamma_0)\,\gamma_1\Big)\,\eta + \gamma_0\,(2\beta_0^2 + 3\,\beta_0\,\gamma_0 + \gamma_0^2)\,\eta^2\Big] \\
& + \frac{1}{24}\,a^4(s^*)\,\eta\Big[-24\,\gamma_3 + 12(\beta_2\,\gamma_0 + 2\beta_1\,\gamma_1 + \gamma_1^2 + 3\,\beta_0\,\gamma_2 + 2\,\gamma_0\,\gamma_2)\,\eta \\
& - 4\Big(6\beta_0^2\,\gamma_1 + 3\,\gamma_0^2\,(\beta_1 + \gamma_1) + \beta_0\,\gamma_0\,(5\,\beta_1 + 9\,\gamma_1)\Big)\,\eta^2 + \gamma_0\,(6\beta_0^3 + 11\,\beta_0^2\,\gamma_0 \\
& + 6\,\beta_0\,\gamma_0^2 + \gamma_0^3)\,\eta^3\Big] \\
& + \frac{1}{120}\,a^5(s^*)\,\eta\Big[-120\,\gamma_4 + \frac{1}{\beta_0}60\Big(-7\,\beta_1\,\beta_2\,\gamma_0 + 4\,\beta_0^2\,\gamma_3 + \beta_0\,(7\,\beta_1\,\gamma_0 + \beta_3\,\gamma_0 \\
& + 2\,\beta_2\,\gamma_1 + 3\,\beta_1\,\gamma_2 + 2\gamma_1\,\gamma_2 + 2\,\gamma_0\,\gamma_3)\Big)\,\eta - 20\Big(3\beta_1^2\,\gamma_0 + \beta_1\,(14\beta_0 + 9\,\gamma_0)\,\gamma_1 \\
& + 3\,(2\beta_0 + \gamma_0)(\beta_2\,\gamma_0 + \gamma_1^2 + 2\,\beta_0\,\gamma_2 + \gamma_0\,\gamma_2)\Big)\,\eta^2 + 10\Big(12\,\beta_0^3\,\gamma_1 + \gamma_0^3(3\,\beta_1 + 2\,\gamma_1) \\
& + \beta_0\,\gamma_0^2\,(13\,\beta_1 + 12\,\gamma_1) + \beta_0^2\,\gamma_0\,(13\,\beta_1 + 22\,\gamma_1)\Big)\,\eta^3 - \gamma_0\Big(24\,\beta_0^4 + 50\,\beta_0^3\,\gamma_0 \\
& + 35\,\beta_0^2\,\gamma_0^2 + 10\,\beta_0\,\gamma_0^3 + \gamma_0^4\Big)\,\eta^4\Big] + O(a^6(s^*))\Big\}
\end{aligned} \tag{8}$$

where $\eta = \ln(s/s^*)$.

This is the updated series expansion of the quark mass renormalization group equation to fifth-loop order. Up to third-loop order Eq.(8) agrees exactly with Kniehl (1996), and up to forth-loop order with Chetyrkin et al. (1997).

For three active quark flavours, substituting the known values of the γ- and β-coefficients into Eq.(8) results in

$$
\begin{aligned}
\overline{m}_q(s) \;=\; & \overline{m}_q(s^*)\Big\{1 - a(s^*)\,\gamma_0\,\eta + a^2(s^*)\Big[\frac{1}{72}\Big(-303 + 10n_f\Big)\eta + \frac{1}{24}\Big(45 - 2n_f\Big)\eta^2\Big] \\
& + a^3(s^*)\Big[\Big(-\frac{1249}{64} + (\frac{277}{216} + \frac{5\zeta_3}{6})n_f + \frac{140}{81}n_f^2\Big)\eta + \Big(\frac{607}{32} - \frac{233}{144}n_f + \frac{5}{216}n_f^2\Big)\eta^2 \\
& + \Big(-\frac{65}{16} + \frac{7}{18}n_f + \frac{1}{108}n_f^2\Big)\eta^3\Big] \\
& + a^4(s^*)\Big[\Big(-98.943 + 19.108n_f - 0.276n_f^2 - 0.006n_f^3\Big)\eta + \Big(-146.861 - 23.571n_f \\
& - 8.120n_f^2 + 0.432n_f^3\Big)\eta^2 + \Big(-69.086 + 9.698n_f - 0.389n_f^2 + 0.004n_f^3\Big)\eta^3 \\
& + \Big(9.395 - 1.407n_f + 0.070n_f^2 - 0.001n_f^3\Big)\eta^4\Big] \\
& + a^5(s^*)\Big[\Big(-559.707 + 143.686n_f - 7.482n_f^2 - 0.108n_f^3 + 0.0001n_f^4\Big)\eta \\
& + \Big(\frac{1}{2n_f - 33}(-29836.577 + 8585.863n_f + 22.617n_f^2 - 98.278n_f^3 + 4.520n_f^4 - 0.004n_f^5)\Big)\eta^2 \\
& + \Big(-775.076 + 164.071n_f + 26.364n_f^2 - 3.556n_f^3 + 0.096n_f^4\Big)\eta^3 \\
& + \Big(230.956 - 45.430n_f + 3.081n_f^2 - 0.082n_f^3 + 0.0006n_f^4\Big)\eta^4 \\
& + \Big(-22.547 + 4.630n_f - 0.356n_f^2 + 0.012n_f^3 - 0.0002n_f^4\Big)\eta^5\Big] \;+\; O(a^6(s^*))\Big\}
\end{aligned} \tag{9}
$$

with ζ_n the Riemann zeta-function, $n_f = 3$ in the light quark sector and $\eta = \ln(s/s^*)$.

4. Evaluating the Accuracy of the Perturbative Series Expansion of $\overline{m}_q(s)$

Eq.(8) is the perturbative series expansion of the running quark mass $\overline{m}_q(s)$ in powers of $\eta = \ln(s/s^*)$, with the initial value $\overline{m}_q(s^*)$ to fifth-loop order. We are now interested in the effect of the latest loop order (i.e. the $O(a^5(s^*))$ term). To do this we compare Eq.(8) with the forth-loop series determined by Chetyrkin et al. (1997). Alternatively, we could directly integrate Eqs.(1)-(2) to find the running coupling $a_s(s)$ and running quark mass $\overline{m}_q(s)$ through numerical means. This is the method employed in RunDec, a Mathematica (and C) package used for the decoupling and running of the strong coupling constant and quark masses developed by Chetyrkin et al. (2000).

Fig.(1) shows the difference between the direct numerical integration of Eq.(2) for the running of $\overline{m}_{ud}(s)$ and i). the perturbative series solution to fifth-loop order Eq.(8), ii). the perturbative series solution to forth-loop order (Chetyrkin et al., 1997). Here we have set the initial mass condition $\overline{m}_{ud}(s^* = (2\,\text{GeV})^2) = (3.9 \pm 0.2)\,\text{MeV}$ (Dominguez et al., 2018), where $\overline{m}_{ud}(s)$ is defined as

$$\overline{m}_{ud}(s) \equiv \frac{\overline{m}_u(s) + \overline{m}_d(s)}{2} \tag{10}$$

We have also made use of the strong coupling constant $a_s((2\,\text{GeV})^2) = 0.098 \pm 0.004$ which is found using the perturbative series expansion of the strong coupling RG equation (Davier et al., 2006) with the initial condition $\alpha_s(m_\tau^2 = 3.16\,\text{GeV}^2) = 0.328 \pm 0.013$ (Pich, 2017).

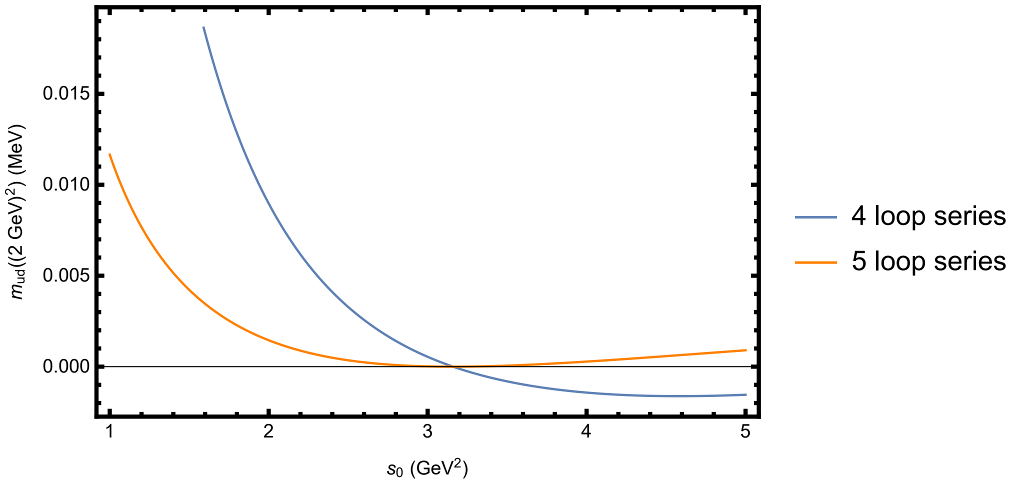

Figure 1: The difference between the direct numerical integration of the quark mass RG equation and i). the fifth-loop series expansion (orange), ii). the forth-loop series expansion (blue).

The direct numerical integration approach can be used as a reference from which we statistically compare how well it is approximated by the forth-loop (Chetyrkin et al., 1997) and by the fifth-loop (Eq.(8)) series expansion.

Varying the energy scale between $1\,\text{GeV}^2$ and $5\,\text{GeV}^2$ in increments of 0.001, describes 4001 points at which to evaluate $\overline{m}_q(s)$, a light quark mass with the initial condition $\overline{m}_q(s^*)$ set equal to 1 MeV. Two common statistical evaluation criteria: Root Mean Absolute Error (RMSE) and Mean Absolute Error (MAE) are used. The Root Mean Absolute Error is defined as RMSE $= \sqrt{\frac{1}{n}\sum_{j=1}^{n}(r_j - k_j)^2}$, and the Mean Absolute Error is calculated as MAE $= \frac{1}{n}\sum_{j=1}^{n}|r_j - k_j|$. Where r_j is our reference i.e. $\overline{m}_q(s)$ calculated by directly numerically integrating Eq.(2) at each point j in the s range described; and k_j is the quark mass $\overline{m}_q(s)$ calculated using the perturbative series solution to either the forth- or fifth-loop order at a particular point j within the s range. The Mean Absolute Error can be interpreted as the average error rate. While the Root Mean Square Error is more sensitive to a large deviation between the function and the reference function at a single point. The MAE and RMSE for the forth- and fifth-loop perturbative series solution are given in Tab.(2). The largest absolute deviation is also given, in order to provide context for the MAE and RMSE values.

From Fig.(1). and the low MAE and RMSE in Tab.(2), we conclude that the fifth-loop perturbative series solution for the quark mass does not deviate significantly from the direct numerical integration of the the mass RG equation. Hence the $O(a_s^5)$ correction to the series solution of the mass RG equation is a valuable addition. We hope that it is evident to the reader how useful Rubi is as a tool for work in the STEM field.

Table 2: Error evaluation for the forth-loop (Chetyrkin et al., 1997) and by the fifth-loop (Eq.(8)) series expansion, using the direct numerical integration of the quark mass RG equation as a reference

Statistic	Fifth-loop series solution	Forth-loop series solution
Mean Abs. Error	0.0004	0.0011
Root Mean Squared Error	0.0471	0.1130
Largest Abs. Deviation	0.0030	0.0070
Smallest Abs. Deviation	0	0

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