Mathematica and Fortran programs for various analytic QCD couplings

César Ayala and Gorazd Cvetič

Department of Physics, Universidad Técnica Federico Santa María, Casilla 110-V, Valparaíso, Chile

E-mail: gorazd.cvetic@gmail.com

Abstract. We outline here the motivation for the existence of analytic QCD models, i.e., QCD frameworks in which the running coupling $\mathcal{A}(Q^2)$ has no Landau singularities. The analytic (holomorphic) coupling $\mathcal{A}(Q^2)$ is the analog of the underlying pQCD coupling $a(Q^2) \equiv \alpha_s(Q^2)/\pi$, and any such $\mathcal{A}(Q^2)$ defines an analytic QCD model. We present the general construction procedure for the couplings $\mathcal{A}_\nu(Q^2)$ which are analytic analogs of the powers $a(Q^2)^\nu$. Three analytic QCD models are presented. Applications of our program (in Mathematica) for calculation of $\mathcal{A}_\nu(Q^2)$ in such models are presented. Programs in both Mathematica and Fortran can be downloaded from the web page: gcvetic.usm.cl.

1. Why analytic QCD?

Perturbative QCD (pQCD) running coupling $a(Q^2)$ [$\equiv \alpha_s(Q^2)/\pi$, where $Q^2 \equiv -q^2$] has unphysical (Landau) singularities at low spacelike momenta $0 < Q^2 \lesssim 1 \ \mathrm{GeV}^2$.

For example, the one-loop pQCD running coupling

$$a(Q^2)^{(1-\ell.)} = \frac{1}{\beta_0 \ln(Q^2/\Lambda^2_{\mathrm{Lan.}})} \tag{1}$$

has a Landau singularity (pole) at $Q^2 = \Lambda^2_{\mathrm{Lan.}}$ ($\sim 0.1 \ \mathrm{GeV}^2$). The 2-loop pQCD coupling $a(Q^2)^{(2-\ell.)}$ has a Landau pole at $Q^2 = \Lambda^2_{\mathrm{Lan.}}$ and Landau cut at $0 < Q^2 < \Lambda^2_{\mathrm{Lan.}}$.

It is expected that the true QCD coupling $\mathcal{A}(Q^2)$ has no such singularities. Why?

General principles of QFT dictate that any spacelike observable $\mathcal{D}(Q^2)$ (correlators of currents, structure functions, etc.) is an analytic (holomorphic) function of Q^2 in the entire Q^2 complex plane with the exception of the timelike axis: $Q^2 \in \mathbb{C}\backslash(-\infty, -M^2_{\mathrm{thr.}}]$, where $M_{\mathrm{thr.}} \sim 0.1$ GeV is a threshold mass ($\sim M_\pi$). If $\mathcal{D}(Q^2)$ can be evaluated as a leading-twist term, then it is a function of the running coupling $a(\kappa Q^2)$ where $\kappa \sim 1$: $\mathcal{D}(Q^2) = \mathcal{F}(a(\kappa Q^2))$. Then the argument $a(\kappa Q^2)$ is expected to have the same analyticity properties as $\mathcal{D}$, which is not the case with the pQCD coupling in the usual renormalization schemes ($\overline{\mathrm{MS}}$, 't Hooft, etc.).

A QCD coupling $\mathcal{A}(Q^2)$ with holomorphic behavior for $Q^2 \in \mathbb{C}\backslash(-\infty, -M^2_{\mathrm{thr.}}]$, represents an analytic QCD model (anQCD).

Such holomorphic behavior comes usually together with (IR-fixed-point) behavior [$\mathcal{A}(0) < \infty$]. The IR-fixed-point behavior of $\mathcal{A}(Q^2)$ is suggested by:

- lattice calculations [1, 2, 3]; calculations based on Dyson-Schwinger equations (DSE) [4, 5]; Gribov-Zwanziger approach [6, 7];

- The holomorphic $\mathcal{A}(Q^2)$ with IR-fixed-point behavior was proposed in various analytic QCD models, among them:
  (i) Analytic Perturbation Theory (APT) of Shirkov, Solovtsov et al. [8, 9, 10, 11, 12];
  (ii) its extension Fractional APT (FAPT) [13, 14, 15];
  (iii) analytic models with $\mathcal{A}(Q^2)$ very close to $a(Q^2)$ at high $|Q^2| > \Lambda^2_{\rm Lan.}$: $\mathcal{A}(Q^2) - a(Q^2) \sim (\Lambda^2_{\rm Lan.}/Q^2)^N$ with $N = 3, 4$ or 5, [16, 17, 18, 19];
  (iv) Massive Perturbation Theory (MPT), [20, 21, 22, 23].

Perturbative QCD (pQCD) can give analytic coupling $a(Q^2)$ in specific schemes with IR fixed point; the condition of reproduction of the correct value of the (strangeless and massless) semihadronic τ lepton $V + A$ decay ratio $r_\tau \approx 0.20$ strongly restricts such schemes [24, 25, 26].

If the analytic coupling $\mathcal{A}(Q^2)$ is not perturbative, $\mathcal{A}(Q^2)$ differs from the pQCD couplings $a(Q^2)$ at $|Q| \gtrsim 1$ GeV by nonperturbative (NP) terms, typically by some power-suppressed terms $\sim 1/Q^{2N}$ or $1/[Q^{2N} \ln^K(Q^2/\Lambda^2_{\rm Lan.})]$.

An analytic QCD model which gives $\mathcal{A}(0) = \infty$ was constructed in [27, 28, 29].

2. The formalism of constructing $\mathcal{A}_\nu$ in general anQCD

Having $\mathcal{A}(Q^2)$ [the analytic analog of $a(Q^2)$] specified, we want to evaluate the physical QCD quantities $\mathcal{D}(Q^2)$ in terms of such $\mathcal{A}(\kappa Q^2)$.

Usually $\mathcal{D}(Q^2)$ is known as a (truncated) power series in terms of the pQCD coupling $a(\kappa Q^2)$:

$$\mathcal{D}(Q^2)^{[N]}_{\rm pt} = a(\kappa Q^2)^{\nu_0} + d_1(\kappa) a(\kappa Q^2)^{\nu_0+1} + \ldots + d_{N-1}(\kappa) a(\kappa Q^2)^{\nu_0+N-1}. \quad (2)$$

In anQCD, the simple replacement $a(\kappa Q^2)^{\nu_0+m} \mapsto \mathcal{A}(Q^2)^{\nu_0+m}$ is not correct, it leads to a strongly diverging series when N increases, as argued in [30]; a different formalism was needed, and was developed for general anQCD, first for the case of integer ν_0 [31, 32], and then for the case of general ν_0 [33]. It results in the replacements

$$a(\kappa Q^2)^{\nu_0+m} \mapsto \mathcal{A}_{\nu_0+m}(Q^2) \quad \left[\neq \mathcal{A}(Q^2)^{\nu_0+m}\right] , \quad (3)$$

where the construction of the analytic power analogs $\mathcal{A}_{\nu_0+m}(Q^2)$ from $\mathcal{A}(Q^2)$ was obtained.

The construction starts with logarithmic derivatives of $\mathcal{A}(Q^2)$ [where $\beta_0 = (11 - 2N_f/3)/4$]:

$$\tilde{\mathcal{A}}_{n+1}(Q^2) \equiv \frac{(-1)^n}{\beta_0^n n!} \left(\frac{\partial}{\partial \ln Q^2} \right)^n \mathcal{A}(Q^2) , \qquad (n = 0, 1, 2, \ldots) , \quad (4)$$

and $\widetilde{\mathcal{A}}_1 \equiv \mathcal{A}$. Using the Cauchy theorem, these quantities can be expressed in terms of the discontinuity function of anQCD coupling $\widetilde{\mathcal{A}}$ along its cut, $\rho(\sigma) \equiv {\rm Im} \mathcal{A}(-\sigma - i\epsilon)$

$$\widetilde{\mathcal{A}}_{n+1}(Q^2) = \frac{1}{\pi} \frac{(-1)}{\beta_0^n \Gamma(n+1)} \int_0^\infty \frac{d\sigma}{\sigma} \rho(\sigma) {\rm Li}_{-n}(-\sigma/Q^2) . \quad (5)$$

This construction can be extended to a general noninteger $n \mapsto \nu$

$$\widetilde{\mathcal{A}}_{\nu+1}(Q^2) = \frac{1}{\pi} \frac{(-1)}{\beta_0^\nu \Gamma(\nu+1)} \int_0^\infty \frac{d\sigma}{\sigma} \rho(\sigma) {\rm Li}_{-\nu}\left(-\frac{\sigma}{Q^2}\right) \quad (-1 < \nu) . \quad (6)$$

This can be recast into an alternative form, involving $\mathcal{A}$ ($\equiv \widetilde{\mathcal{A}}_1$) instead of ρ

$$\tilde{\mathcal{A}}_{\delta+m}(Q^2) \;\; = \;\; K_{\delta,m} \left(\frac{d}{d \ln Q^2} \right)^m \int_0^1 \frac{d\xi}{\xi} \mathcal{A}(Q^2/\xi) \ln^{-\delta}\left(\frac{1}{\xi}\right) , \quad (7)$$

where: $0 \leq \delta < 1$ and $m = 0, 1, 2, \ldots$; $K_{\delta,m} = (-1)^m \beta_0^{-\delta-m+1}/[\Gamma(\delta+m)\Gamma(1-\delta)]$. This expression was obtained from Eq. (6) by the use of the following expression for the $\mathrm{Li}_{-\nu}(z)$ function [34]:

$$\mathrm{Li}_{-n-\delta}(z) = \left(\frac{d}{d\ln z}\right)^{n+1} \left[\frac{z}{\Gamma(1-\delta)} \int_0^1 \frac{d\xi}{1-z\xi} \ln^{-\delta}\left(\frac{1}{\xi}\right)\right] \quad (n = -1, 0, 1, \ldots; 0 < \delta < 1) \ . \tag{8}$$

The analytic analogs $\mathcal{A}_\nu$ of powers a^ν are then obtained by combining various generalized logarithmic derivatives (with the coefficients $\widetilde{k}_m(\nu)$ obtained in [33])

$$\mathcal{A}_\nu = \widetilde{\mathcal{A}}_\nu + \sum_{m \geq 1} \widetilde{k}_m(\nu) \widetilde{\mathcal{A}}_{\nu+m} \ . \tag{9}$$

3. The considered anQCD models

We constructed Mathematica and Fortran programs for three anQCD models: 1.) Fractional Analytic Perturbation Theory (FAPT) [13, 14, 15]; 2.) 2δ analytic QCD (2δanQCD) [19]; 3.) Massive Perturbation Theory (MPT) [20, 21, 22, 23]. These three models are described below.

3.1. anQCD models: FAPT

Application of the Cauchy theorem to the function $a(Q'^2)^\nu/(Q'^2 - Q^2)$ gives

$$a(Q^2)^\nu = \frac{1}{\pi} \int_{\sigma=-\Lambda^2_{\mathrm{Lan.}}-\eta}^{\infty} \frac{d\sigma \mathrm{Im}(a(-\sigma - i\epsilon)^\nu)}{(\sigma + Q^2)}, \quad (\eta \to +0). \tag{10}$$

In FAPT, the integration over the Landau part of the cut in the above integral is eliminated; since $\sigma \equiv -Q^2$, the Landau cut is $-\Lambda^2_{\mathrm{Lan.}} < \sigma < 0$. This leads to the FAPT coupling

$$\mathcal{A}_\nu^{(\mathrm{FAPT})}(Q^2) = \frac{1}{\pi} \int_{\sigma=0}^{\infty} \frac{d\sigma \mathrm{Im}(a(-\sigma - i\epsilon)^\nu)}{(\sigma + Q^2)} \ . \tag{11}$$

3.2. anQCD models: 2δQCD

Here, $\rho(\sigma) \equiv \mathrm{Im}\mathcal{A}(-\sigma - i\epsilon)$ is approximated at high momenta $\sigma \geq M_0^2$ by $\rho^{(\mathrm{pt})}(\sigma)$ [$\equiv \mathrm{Im}\ a(-\sigma - i\epsilon)$], and in the unknown low-momentum regime by two deltas:

$$\rho^{(2\delta)}(\sigma) = \pi F_1^2 \delta(\sigma - M_1^2) + \pi F_2^2 \delta(\sigma - M_2^2) + \Theta(\sigma - M_0^2)\rho^{(\mathrm{pt})}(\sigma) \quad \Rightarrow \tag{12}$$

$$\widetilde{\mathcal{A}}_\nu^{(2\delta)}(Q^2) = \frac{(-1)}{\beta_0^\nu \Gamma(\nu+1)} \left\{ \sum_{j=1}^{2} \frac{F_j^2}{M_j^2} \mathrm{Li}_{-\nu}\left(-\frac{M_j^2}{Q^2}\right) + \frac{1}{\pi}\int_{M_0^2}^{\infty} \frac{d\sigma}{\sigma} \mathrm{Im} a(-\sigma - i\epsilon) \mathrm{Li}_{-\nu}\left(-\frac{\sigma}{Q^2}\right)\right\}. \tag{13}$$

The parameters F_j^2 and M_j ($j = 1, 2$) are fixed in such a way that the resulting deviation from the underlying pQCD at high $|Q^2| > \Lambda^2$ is: $\mathcal{A}_\nu^{(2\delta)}(Q^2) - a(Q^2)^\nu \sim (\Lambda^2/Q^2)^5$. The pQCD-onset scale M_0 is determined so that the model reproduces the measured (strangeless and massless) $V + A$ tau lepton semihadronic decay ratio $r_\tau \approx 0.20$.

The underlying pQCD coupling a is chosen in 2δanQCD, for calculational convenience, in the Lambert-scheme form

$$a(Q^2) = -\frac{1}{c_1} \frac{1}{1 - c_2/c_1^2 + W_{\mp 1}(z_\pm)} \ , \tag{14}$$

where: $c_1 = \beta_1/\beta_0$; $Q^2 = |Q^2| e^{i\phi}$, the upper (lower) sign when $\phi \geq 0$ ($\phi < 0$), and

$$z_\pm = (c_1 \mathrm{e})^{-1} (|Q^2|/\Lambda^2)^{-\beta_0/c_1} \exp\left[i(\pm\pi - \beta_0\phi/c_1)\right]. \tag{15}$$

3.3. anQCD models: MPT

Nonperturbative physics suggests that the gluon acquires at low momenta an effective (dynamical) mass $m_{\rm gl} \sim 1$ GeV, and that the coupling then has the form

$$\mathcal{A}^{(\rm MPT)}(Q^2) = a(Q^2 + {m_{\rm gl}}^2) \ . \tag{16}$$

Since $m_{\rm gl} > \Lambda_{\rm Lan.}$, the new coupling has no Landau singularities.

The (generalized) logarithmic derivatives $\widetilde{\mathcal{A}}^{(\rm MPT)}_{\delta+m}(Q^2)$ are then uniquely determined

$$\widetilde{\mathcal{A}}_{\delta+m}(Q^2) = K_{\delta,m} \left(\frac{d}{d \ln Q^2} \right)^m \int_0^1 \frac{d\xi}{\xi} \mathcal{A}^{(\rm MPT)}(Q^2/\xi) \ln^{-\delta}\left(\frac{1}{\xi}\right) . \tag{17}$$

4. Numerical implementation and results

Programs of numerical implementation in anQCD models:

- for integer power analogs $\mathcal{A}_n(Q^2)$ in APT and in "massive QCD" [35, 36]: Nesterenko and Simolo, 2010 (in Maple) [37], and 2011 (in Fortran) [38];
- for general power analogs $\mathcal{A}_\nu(Q^2)$ in FAPT: Bakulev and Khandramai, 2013 (in Mathematica) [39];
- for general power analogs $\mathcal{A}_\nu(Q^2)$ in 2δanQCD, MPT and FAPT: the presented work in Mathematica [40] and Fortran (programs in both languages can be downloaded from the web page: **gcvetic.usm.cl**).

The basic relations for the numerical implementation of $\mathcal{A}_\nu$ are: in FAPT Eq. (11); in 2δanQCD Eqs. (13) and (9); in MPT Eqs. (17) and (9).

In Mathematica, ${\rm Li}_{-\nu}(z)$ is implemented as PolyLog$[-\nu, z]$. In Mathematica 9.0.1 it is unstable for $|z| \gg 1$. Therefore, we provide a subroutine Li_nu.m (which is called by the main Mathematica program anQCD.m) and gives a stable version under the name polylog$[-\nu, z]$. This problem does not exist in Mathematica 10.0.1.

In Fortran, program Vegas [41] is used for integrations. However, in Fortran, ${\rm Li}_{-\nu}(z)$ function is not implemented for general (complex) z, and is evaluated as an integral Eq. (8). Therefore, the evaluation of $\widetilde{\mathcal{A}}_\nu$'s in 2δanQCD is somewhat more time consuming in Fortran than in Mathematica. Further, more care has to be taken in Fortran to deal correctly with singularities of the integrands.

5. Main procedures in Mathematica for three analytic QCD models

1.) AFAPTNl$[N_f, \nu, 0, |Q^2|, \Lambda^2, \phi]$ gives N-loop ($N = 1,2,3,4$) analytic FAPT coupling $\mathcal{A}_\nu^{({\rm FAPT},N)}(Q^2, N_f)$ with real power index ν, with fixed number of active quark flavors N_f, in the Euclidean domain $[Q^2 = |Q^2| \exp(i\phi) \in \mathcal{C}$ and $Q^2 \not< 0]$

$$\begin{aligned} {\rm AFAPT}N{\rm l}[Nf, \nu, 0, Q2, L2, \phi] &= \mathcal{A}_\nu^{({\rm FAPT},N)}[Q2 = |Q^2|, \phi = \arg(Q^2); Nf = N_f; L2 = \overline{\Lambda}^2_{N_f}] \\ & (N = 1,2,3,4 ;\ Nf = 3,4,5,6). \end{aligned}$$

2.) A2dNl$[N_f, M, \nu, |Q^2|, \phi]$ gives "N-loop" 2δanQCD coupling $\mathcal{A}^{(2\delta)}_{\nu+M}(Q^2, N_f)$, with power index $\nu + M$ ($\nu > -1$ and real; $M = 0, 1, \ldots, N-1$), with number of active quark flavors N_f, in the Euclidean domain. It is used in the N^{N-1}LO truncation approach [where in (9): $\nu_0 \mapsto \nu$ and $n \mapsto M$, and we truncate at $\widetilde{\mathcal{A}}_{\nu+N-1}$]

$$\begin{aligned} {\rm A2d}N{\rm l}[Nf, M, \nu, Q2, \phi] &= \mathcal{A}^{(2\delta)}_{\nu+M}[Q2 = |Q^2|, \phi = \arg(Q^2); Nf = N_f] , \\ & (N = 1,2,3,4,5;\ Nf = 3,4,5,6;\ M = 0,1,\ldots,N-1). \end{aligned}$$

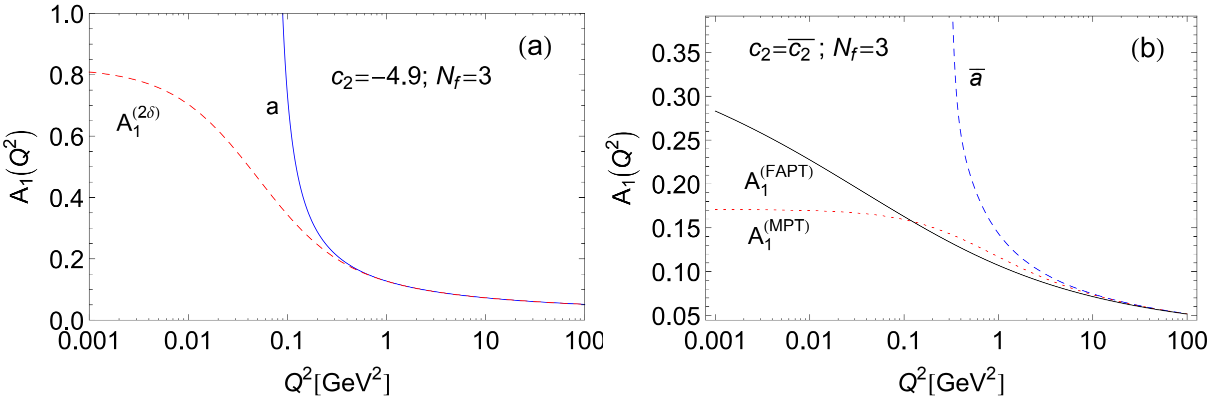

Figure 1. $\mathcal{A}_1 \equiv \mathcal{A}$ in three anQCD models with $\nu = 1$ and $N_f = 3$, as a function of Q^2 for $Q^2 > 0$; the underlying pQCD coupling a is included for comparison: (a) 2δanQCD coupling and pQCD coupling, in the Lambert scheme with $c_2 = -4.9$ (and $c_j = c_2^{j-1}/c_1^{j-2}$ for $j \geq 3$); (b) FAPT and MPT in 4-loop $\overline{\rm MS}$ scheme and with $\overline{\Lambda}_3^2 = 0.1$ GeV^2; MPT is with $m_{\rm gl}^2 = 0.7$ GeV^2.

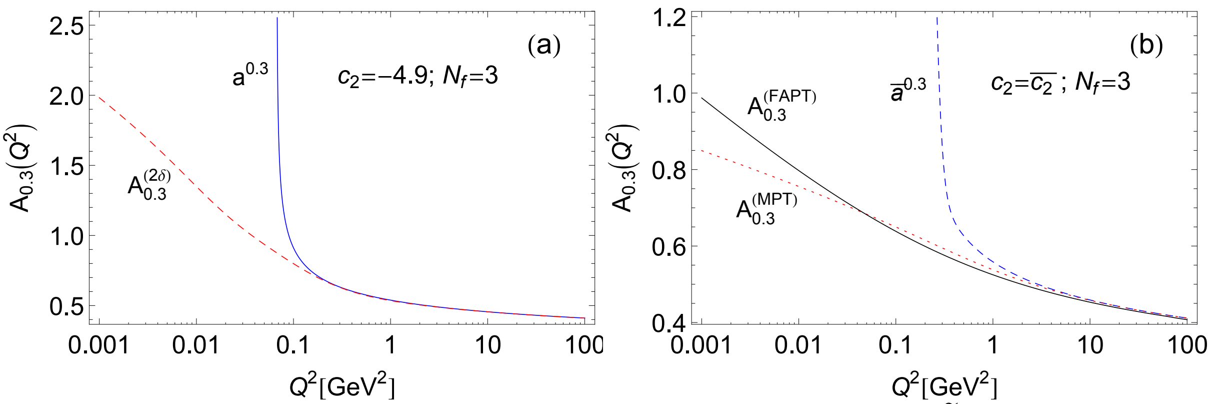

Figure 2. The same as in Fig. 1, but with $\nu = 0.3$ ($\mathcal{A}_{\nu=0.3}$). $\mathcal{A}_{0.3}$ is calculated from $\widetilde{\mathcal{A}}_{0.3+m}$ using the relation (9) with $\nu_0 = 0.3$, and truncation at $\widetilde{\mathcal{A}}_{0.3+4}$ in 2δanQCD, and at $\widetilde{\mathcal{A}}_{0.3+3}$ in MPT; and in FAPT using Eq. (11). Figs. 1 and 2 are taken from [40].

3.) AMPTNl$[N_f, \nu, Q^2, {m_{\rm gl}}^2, \overline{\Lambda}_{N_f}^2]$ gives N-loop ($N = 1, 2, 3, 4$) analytic MPT coupling $\mathcal{A}_{\nu}^{({\rm MPT},N)}(Q^2, {m_{\rm gl}}^2, N_f)$, with real power index ν ($0 < \nu < 5$) and with number of active quark flavors N_f, in the Euclidean domain ($Q^2 \in \mathcal{C}$ and $Q^2 \nless 0$)

$$\begin{aligned} {\rm AMPT}N{\rm l}[Nf, \nu, Q2, M2, L2] \;&=\; \mathcal{A}_{\nu}^{(\rm MPT,N)}[Q2 = Q^2 \in \mathcal{C}; Nf = N_f; M2 = {m_{\rm gl}}^2; L2 = \overline{\Lambda}_{N_f}^2] \\ & (N = 1, 2, 3, 4;\; Nf = 3, 4, 5, 6);\; 0 < \nu < 5). \end{aligned} \tag{18}$$

Examples:
Input scale of the underlying $\overline{\rm MS}$ pQCD for FAPT and MPT is $\overline{\Lambda}_3^2 = 0.1$ GeV^2. The times are for a typical laptop, using Mathematica 9.0.1; the first entry in the results is the time of calculation, in s.

In[1]:= <<anQCD.m;
In[2]:= AFAPT3l[5, 1, 0, 10^2, 0.1, 0] // Timing
Out[2]= {0.382942, 0.0624843}
In[3]:= AMPT3l[5, 1, 10^2, 0.7, 0.1] // Timing
Out[3]= {0.108983, 0.0627726}

In[4]:= A2d3l[5, 0, 1, 10^2, 0] // Timing
Out[4]=$\{0.768884, 0.0559182\}$
In[5]:= AFAPT3l[3, 1, 0, 0.5, 0.1, 0] // Timing
Out[5]= $\{0.378943, 0.121853\}$
In[6]:= AMPT3l[3, 1, 0.5, 0.7, 0.1] // Timing
Out[6]= $\{0.106984, 0.132199\}$
In[7]:= A2d3l[3, 0, 1, 0.5, 0] // Timing
Out[7]= $\{0.775882, 0.163402\}$
In[8]:= AFAPT3l[3, 0.3, 0, 0.5, 0.1, 0] // Timing
Out[8]= $\{0.456930, 0.556644\}$
In[9]:= AMPT3l[3, 0.3, 0.5, 0.7, 0.1] // Timing
Out[9]=$\{0.110983, 0.569473\}$
In[10]:= A2d3l[3, 0, 0.3, 0.5, 0] // Timing
Out[10]= $\{3.125525, 0.576005\}$

6. Conclusions

We constructed programs, in Mathematica and Fortran, which evaluate couplings $\mathcal{A}_\nu(Q^2)$ in three models of analytic QCD (FAPT, 2δanQCD, and MPT). These couplings are holomorphic functions (free of Landau singularities) in the complex Q^2 plane with the exception of the negative semiaxis, and are analogs of powers $a(Q^2)^\nu \equiv (\alpha_s(Q^2)/\pi)^\nu$ of the underlying perturbative QCD. We checked that our results in FAPT model agree with those of Mathematica program [39].

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