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`anQCD`: `Fortran` programs for couplings at complex momenta in various analytic QCD models

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Abstract

We provide three `Fortran` programs which evaluate the QCD analytic (holomorphic) couplings $\mathcal{A}_\nu(Q^2)$ for complex or real squared momenta Q^2. These couplings are holomorphic analogs of the powers $a(Q^2)^\nu$ of the underlying perturbative QCD (pQCD) coupling $a(Q^2) \equiv \alpha_s(Q^2)/\pi$, in three analytic QCD models (anQCD): Fractional Analytic Perturbation Theory (FAPT), Two-delta analytic QCD (2δanQCD), and Massive Perturbation Theory (MPT). The index ν can be noninteger. The provided programs do basically the same job as the `Mathematica` package `anQCD.m` published by us previously, Ref. [1], but are now written in `Fortran`.

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Program Summary

TProgram titles: `AFAPText.for, A2danQCDext.for, AMPText.for`

The main programs (`AFAPText.for, A2danQCDext.for, AMPText.for`*) and the tar-gzipped file containing all three programs and this text (*`AanQCDextFOR.tar.gz`*), available from the web page:*
`gcvetic.usm.cl`

Computer: Any work-station or PC where `Fortran 95/2003/2008` (gfortran) is running

Operating system in which the program has been tested: Operating system Linux (Ubuntu and Scientific Linux), Windows (in all cases using gfortran)

No. of bytes in distributed programs:
103 kB (`AFAPText.for`), 107 kB (`A2danQCDext.for`), 236 kB (`AMPText.for`); 250 kB (`AanQCDextFOR.tar.gz`)

Distribution format: tar.gz

Keywords: Analytic (holomorphic) QCD coupling, Fractional Analytic Perturbation Theory, Two-delta analytic QCD model, Massive Perturbation Theory, Perturbative QCD, Renormalization group evolution.

Nature of problem: Calculation of values of the running analytic couplings $\mathcal{A}_\nu(Q^2; N_f)$ for general complex squared momenta $Q^2 \equiv -q^2$, in three analytic QCD models, where $\mathcal{A}_\nu(Q^2; N_f)$ is the analytic (holomorphic) analog of the power $(\alpha_s(Q^2; N_f)/\pi)^\nu$. Here, $\mathcal{A}_\nu(Q^2; N_f)$ is a holomorphic function in the Q^2 complex plane, with the exception of the negative semiaxis $(-\infty, -M^2_{\rm thr})$, reflecting the analiticity properties of the spacelike renormalization invariant quantities $\mathcal{D}(Q^2)$ in QCD. In contrast, the perturbative QCD power $(\alpha_s(Q^2; N_f)/\pi)^\nu$ has singularities even outside the negative semiaxis (Landau ghosts). The three considered models are: Analytic Perturbation theory (APT); Two-delta analytic QCD (2δanQCD); Massive Perturbation Theory (MPT). We refer to Ref. [1] for more details and literature.

Solution method: The `Fortran` programs for FAPT and 2δanQCD models contain routines and functions needed to perform two-dimensional numerical integrations involving the spectral function, in order to evaluate $\mathcal{A}_\nu(Q^2)$ couplings. In MPT model, one-dimensional numerical integration involving $\mathcal{A}_1(Q^2)$ is sufficient to evaluate any $\mathcal{A}_\nu(Q^2)$ coupling.

Restrictions: For unphysical choices of the input parameters the results are meaningless. When Q^2 is close to the cut region of the couplings (Q^2 real negative), the calculations can take more time and can have less precision.

Running time: For evaluation of a set of about 10 related couplings, the times vary in the range $t \sim 10^1$-10^2 s. MPT requires less time, $t \sim 1$-10^1 s.

1. General remarks

The included `Fortran` programs evaluate the holomorphic couplings $\mathcal{A}_\nu(Q^2)$ in the dispersive approach to QCD, where we consider three analytic versions: Fractional Analytic Perturbation Theory (FAPT) [2] (and references therein), 2δ analytic QCD (2δanQCD) [3] (cf. also [1, 4]), and Massive Perturbation Theory (MPT) [5] (cf. also [6, 7]). These programs are constructed for complex squared momenta $Q^2 \equiv -q^2$, in a similar way as the previously published Mathematica package anQCD.m, Ref. [1].[1] For additional details on the three analytic QCD models with a view to implementing them numerically in Mathematica, we refer to Ref. [1].

A complication appears in `Fortran`, though, because in the dispersion integrals for FAPT and 2δanQCD couplings the polylogarithm function $\mathrm{Li}_\nu(z)$ for complex z appears and it has not been implemented in `Fortran` yet (in `Mathematica` it is implemented as PolyLog$[-\nu, z]$). In the attached `Fortran` programs this function is calculated as the following integral [14]:

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

where $\nu = n + \delta$. For better stability, the numerical integration of this integral over ξ is implemented in the complex plane along a ray in the first quadrant. This then results in two-dimensional integration for the evaluation of FAPT and 2δanQCD couplings $\mathcal{A}_\nu(Q^2)$. This integration is performed numerically with vegas routine [15]. In this approach, overflow and/or underflow problems appear at the edges of the unit square of integration, which are dealt with carefully in the programs. In the evaluation of couplings $\mathcal{A}_\nu(Q^2)$ in MPT model, one-dimensional integrations are needed because the integrand involves $\mathcal{A}_1(Q^2/\xi)$ and no functions $\mathrm{Li}_\nu(z)$.

The `Fortran` programs are self-contained, i.e., no additional packages are needed. The needed explanations and instructions on the input parameters, compiling commands, and the output form, are all given at the beginning of each `Fortran` program. The calculations are more time-consuming in FAPT when the complex squared momenta Q^2 are close to the cut negative semiaxis. In all models (FAPT, 2δanQCD, MPT), the number of active quark flavors N_f is a fixed input integer.

We wish to point out that this program, in `Mathematica` form [1], was already applied without problems to the evaluation of the nonsinglet structure function F_2 in deep inelastic scattering in FAPT model [16].

[1] The analogous `Fortran` programs, but only for real values of the squared momenta Q^2, were mentioned in Ref. [8] (and were made available on the web page: gcvetic.usm.cl). The `Fortran` program for the couplings $A_n(Q^2)$ for integer index n and real Q^2 in APT [9] and massive APT (MAPT) [10] was provided in Ref. [11], based on the corresponding program in Maple [12]. The Mathematica program for evaluation of the general power analogs $\mathcal{A}_\nu(Q^2)$ in FAPT was provided in Ref. [13].

2. Practical aspects of the program

2.1. Input parameters

The programs can get compiled with the simple "gfortran" command. For example, the program A2danQCDext.for can get compiled by writing in the directory where the program is stored: "gfortran -o A2dan A2danQCDext.for" and then executed with the command "./A2dan". Before compiling, however, the input parameters should be typed into the program, at (two) places which start with the string "INPUT". In all three programs the following input parameters need to be specified:

1. N_f ("Nf"), the number of active quarks;
2. $N_{\rm in}$ ("Nin") and $\delta_{\rm in}$ ("delin") indices, where $\nu = N_{\rm in} + \delta_{\rm in}$ is the index of the coupling $\mathcal{A}_\nu$; where $N_{\rm in} = 0, 1, 2, 3, 4$; and $0 \le \delta_{\rm in} \le 1$.
3. $|Q^2|$ ("AbsQ2", in GeV^2) and ϕ ("ArgQ2", in radians), where $Q^2 = |Q^2| \exp(i\phi)$ is the (complex) squared momentum ($Q^2 \equiv -q^2$).

In addition, in the programs AFAPText.for and AMPText.for, the scale $\overline{\Lambda}_{N_f}$ ("gL2MS", in GeV) of the underlying pQCD coupling needs to be specified.

Further, in AMPText.for, the MPT squared effective mass of the gluon $m_{\rm gl}^2$ ("gM2", in GeV^2) needs to be specified. This mass is of the order of magnitude $m_{\rm gl}^2 \sim 1$ GeV^2 [5–7], and is assumed in our program AMPText.for to be constant at all momenta (and thus independent of Q^2 and of N_f). Instead of the input scale $\overline{\Lambda}_{N_f}$ in MPT, which basically determines the strength of the MPT coupling $\mathcal{A}_1^{\rm (MPT)}(Q^2) = \alpha_s(Q^2 + m_{\rm gl}^2; \overline{\rm MS})/\pi$, one might prefer to use the value of $\pi \mathcal{A}_1(M_Z^2) = \alpha_s(M_Z^2 + m_{\rm gl}^2; \overline{\rm MS})$. This then determines the value of the scale $\overline{\Lambda}_{N_f=5}$. The values of other scales $\overline{\Lambda}_{N_f}$ (for $N_f = 4, 3, 6$) can then be obtained by applying the (3-loop) quark threshold relations [17] applied within the (analytic) MPT model

$$\begin{aligned} \mathcal{A}_1' &= \mathcal{A}_1 - \mathcal{A}_2 \frac{\ell_h}{6} + \mathcal{A}_3 \left(\frac{\ell_h^2}{36} - \frac{19}{24} \ell_h + \widetilde{c}_2 \right) \\ &\quad + \mathcal{A}_4 \left[-\frac{\ell_h^3}{216} - \frac{131}{576} \ell_h^2 + \frac{\ell_h}{1728} \left(-6793 + 281(N_f - 1) \right) + \widetilde{c}_3 \right] . \end{aligned} \tag{2}$$

Here, $\mathcal{A}_1' \equiv \mathcal{A}_1^{\rm (MPT)}(\mu_{N_f}^2; N_f - 1)$ and $\mathcal{A}_n \equiv \mathcal{A}_n^{\rm (MPT)}(\mu_{N_f}^2; N_f)$, and $\ell_h = \ln[\mu_{N_f}^2/\overline{m}_q^2] = \ln \kappa$ where $\overline{m}_q = \overline{m}_q(\overline{m}_q)$ is the $\overline{\rm MS}$ mass of the corresponding quark entering at the threshold squared momentum $\mu_{N_f}^2 = \kappa \overline{m}_q^2$ ($\kappa \sim 1$). We recall that in MPT (and FAPT) we use for the underlying pQCD coupling the 4-loop $\overline{\rm MS}$ running coupling. In Table 1 we present the values of the scales $\overline{\Lambda}_{N_f}$ corresponding to various values of $m_{\rm gl}^2$ and $\pi \mathcal{A}_1(M_Z^2)$ in MPT. A similar Table for the values of the scales $\overline{\Lambda}_{N_f}$ was given for FAPT in Ref. [1] (Table 1 there).

In A2danQCD.for program for 2δanQCD model, the scheme parameter c_2 ($= \beta_2/\beta_0$) was set equal to the central preferred value $c_2 = -4.9$ (cf. Table 2 of Ref. [1]).

Table 1: The scales $\overline{\Lambda}_{N_f}$, written in MeV, in MPT analytic model, for various values of $m^2_{\rm gl}$ and $\pi {\mathcal A}_1^{\rm (MPT)} = \alpha_s(M_Z^2 + m^2_{\rm gl}; \overline{\rm MS})$. The threshold parameter $\kappa = 2$ was taken; in parentheses, the results with the threshold parameter $\kappa = 1$ are given.

$m^2_{\rm gl}$ [GeV^2]	$\pi {\mathcal A}_1^{\rm (MPT)}(M_Z^2)$	$\overline{\Lambda}_6$	$\overline{\Lambda}_5$	$\overline{\Lambda}_4$	$\overline{\Lambda}_3$
0.5	0.118	88.3 (88.4)	208.6 (208.6)	291.5 (291.0)	339.8 (338.4)
1.0	0.118	88.3 (88.4)	208.6 (208.6)	291.8 (291.3)	343.1 (342.1)
1.5	0.118	88.3 (88.4)	208.7 (208.7)	292.1 (291.7)	346.5 (345.4)
0.5	0.120	99.8 (99.8)	232.9 (232.9)	321.8 (321.2)	371.1 (369.5)
1.0	0.120	99.8 (99.8)	233.0 (233.0)	322.1 (321.6)	374.8 (373.6)
1.5	0.120	99.8 (99.9)	233.0 (233.0)	322.5 (321.9)	378.5 (377.2)
0.5	0.122	112.3 (112.4)	259.1 (259.1)	354.0 (353.3)	404.2 (402.1)
1.0	0.122	112.3 (112.4)	259.1 (259.1)	354.4 (353.8)	408.0 (406.7)
1.5	0.122	112.3 (112.4)	259.1 (259.1)	354.8 (354.2)	412.1 (410.6)

2.2. Output

After the execution of the program, the results of each program are written in the output file `AFAPText.dat` (or: `A2danQCDext.dat`, `AMPText.dat`). If the input index is $\nu = N + \delta$ ($N = 0, 1, 2, 3$ or 4; and $0 \le \delta \le 1$), the output will consist of the following couplings:

$$\widetilde{\mathcal A}_{N+\delta}(Q^2),\ \widetilde{\mathcal A}_{N+1+\delta}(Q^2),\ \ldots,\ \widetilde{\mathcal A}_{4+\delta}(Q^2), \tag{3a}$$

$$\mathcal{A}_{N+\delta}(Q^2)(\mathrm{N}^N\mathrm{LO}),\ \mathcal{A}_{N+\delta}(Q^2)(\mathrm{N}^{N+1}\mathrm{LO}),\ \ldots, \mathcal{A}_{N+\delta}(Q^2)(\mathrm{N}^4\mathrm{LO}). \tag{3b}$$

Here we recall that $\widetilde{\mathcal A}_\nu(Q^2)$ are the logarithmic derivatives analytically extended to non-integer index $n \mapsto \nu$, where for integer n these derivatives are

$$\widetilde{\mathcal A}_n(Q^2) \equiv \frac{(-1)^{n-1}}{\beta_0^{n-1}(n-1)!} \left(\frac{\partial}{\partial \ln Q^2}\right)^{n-1} \mathcal{A}_1(Q^2)\ , \qquad (n = 1, 2, \ldots)\ . \tag{4}$$

The couplings $\widetilde{\mathcal A}_\nu(Q^2)$ are analytic (holomorphic) in Q^2, and perturbatively we have $\widetilde{\mathcal A}_\nu \sim (\alpha_s(Q^2)/\pi)^\nu$. Further, the couplings $\mathcal{A}_\nu(Q^2)$ are the analytic (holomorphic) analogs of the powers $(\alpha_s(Q^2)/\pi)^\nu$, and they are linear combination of the couplings $\widetilde{\mathcal A}_{\nu+K}(Q^2)$ ($K = 0, 1, \ldots$). For example, $\mathcal{A}_{N+\delta}(Q^2)$ at $\mathrm{N}^{N+M}\mathrm{LO}$ precision (N is integer; $0 \le \delta \le 1$) is the following linear combination:

$$\mathcal{A}_{N+\delta}(Q^2) \ = \ \widetilde{\mathcal A}_{N+\delta}(Q^2) + \sum_{m=1}^{M} \widetilde{k}_m(N+\delta) \widetilde{\mathcal A}_{N+m+\delta}(Q^2). \tag{5}$$

The expressions for the general coefficients $\widetilde{k}_m(N+\delta)$ were obtained in Ref. [18]. These coefficients involve the Euler Ψ function $\Psi(\nu) = (d/d\nu)\Gamma(\nu)$ and its derivatives $\Psi^{(m)}(\nu)$.

In `Fortran`, $\Psi(\nu)$ and $\Psi^{(m)}(\nu)$ are calculated by the routine [19] which is used in our `Fortran` programs.

Here we provide, for illustration, an explicit example of output for the program AMPText.for. Let us take the case where the input parameters are: $m_{\rm gl}^2 = 0.7$ GeV^2, $N_f = 3$, $\overline{\Lambda}_{N_f}^2 = 0.1$ GeV^2; and $N_{\rm in} = 0$, $\delta_{\rm in} = 0.7$, $|Q^2| = 0.8$ GeV^2, $\phi = 1.1$. These data are typed into the program at two places, each of those places starting with a commented string 'INPUT'. In the program, the quantities $m_{\rm gl}^2$, N_f and $\overline{\Lambda}_{N_f}$ are the symbols 'gM2', 'Nf' and 'gL2', respectively; and the parameters $N = N_{\rm in}$, $\delta = \delta_{\rm in}$, $|Q^2|$ and ϕ are the symbols 'Nin', 'deltain', 'AbsQ2' and 'ArgQ2', respectively. The program is then compiled and executed as described in the previous Subsection. The output is generated in the new file AMPText.dat, which has then the following output:

```
Nf= 3   MPT(Nf)=mQCD(Nf):
Lambda^2(MSbar,Nf)=0.100000E+00 GeV^2  M^2_{gluon}=0.700000E+00 GeV^2
ziMIN=0.200000E+00 ziMAX=0.100000E+01

N=  0   del=  0.7000
Abs[Q2]=0.800000E+00 GeV^2 Arg[Q2]=0.110000E+01 radians

A_{N+del}(Q2)(N0LO):   Re=0.227612E+00 Im=-.426739E-01
A_{N+del}(Q2)(N1LO):   Re=0.234727E+00 Im=-.436878E-01
A_{N+del}(Q2)(N2LO)    Re=0.234647E+00 Im=-.437757E-01
A_{N+del}(Q2)(N3LO)    Re=0.234425E+00 Im=-.435684E-01
A_{N+del}(Q2)(N4LO):   Re=0.235215E+00 Im=-.432293E-01

(tilde A)_{N+del}(Q2): Re=0.227611E+00 Im=-.426715E-01

(tilde A)_{del}(Q2):   Re=0.227612E+00 Im=-.426739E-01
(tilde A)_{1+del}(Q2): Re=0.266876E-01 Im=-.380292E-02
(tilde A)_{2+del}(Q2): Re=0.145413E-02 Im=0.160013E-02
(tilde A)_{3+del}(Q2): Re=-.342313E-03 Im=0.319822E-03
(tilde A)_{4+del}(Q2): Re=-.819474E-04 Im=-.351718E-04
A_{N+del}(Q2)=MPT analog of (alpha_s(Q2)/Pi)^(N+del)
```

In the above text, 'ziMIN' and 'ziMAX' are the boundaries in the vegas integration assigned automatically by the program. Further, the (complex) values of $\widetilde{\mathcal{A}}_{K+\delta}(Q^2)$ for $K = 0, 1, 2, 3, 4$ are given, as well as the complex values of $\mathcal{A}_{N+\delta}(Q^2)$=$\mathcal{A}_{0.7}(Q^2)$ at N^{0}LO, N^{1}LO, ..., N^{4}LO [cf. also Eq. (5)].

On the other hand, if $Q^2 > 0$, we write in the program 'ArgQ2=0' (not: 'ArgQ2=0.d0' or other similar forms). In that case, the output couplings will be real.

In the other two programs (A2danQCDext.for, AFAPText.for), the procedure and the

output is completely analogous.

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