Global Fits to Electroweak Data Using GAPP

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At Run II of the Tevatron it will be possible to measure the W boson mass with a relative precision of about 2×10^{-4}, which will eventually represent the best measured observable beyond the input parameters of the SM. Proper interpretation of such an ultrahigh precision measurement, either within the SM or beyond, requires the meticulous implementation and control of higher order radiative corrections. The FORTRAN package GAPP, described here, is specifically designed to meet this need and to ensure the highest possible degrees of accuracy, reliability, adaptability, and efficiency.

1. PRECISION TESTS

Precision analysis of electroweak interactions follows three major objectives: high precision tests of the SM; the determination of its fundamental parameters; and studies of indications and constraints of possible new physics beyond the SM, such as supersymmetry or new gauge bosons. Currently, the experimental information comes from the very high precision Z boson measurements at LEP 1 and the SLC, direct mass measurements and constraints from the Tevatron and LEP 2, and low energy precision experiments, such as in atomic parity violation, ν scattering, and rare decays. These measurements are compared with the predictions of the SM and its extensions. The level of precision is generally very high. Besides the need for high-order loop calculations, it is important to utilize efficient renormalization schemes and scales to ensure sufficient convergence of the perturbative expansions.

The tasks involved called for the creation of a special purpose FORTRAN package, GAPP, short for the *Global Analysis of Particle Properties* [1]. It is mainly devoted to the calculation of pseudo-observables, i.e., observables appropriately idealized from the experimental reality. The reduction of raw data to pseudo-observables is performed by the experimenters with available packages (e.g., ZFITTER for Z pole physics). For cross section and asymmetry measurements at LEP 2 (not implemented in the current version, GAPP_99.7), however, this reduction is not optimal and convoluted expressions should be used instead. GAPP attempts to gather all available theoretical and experimental information; it allows the addition of extra parameters describing new physics; it treats all relevant SM inputs as global fit parameters; and it can easily be updated with new calculations, data, observables, or fit parameters. For clarity and speed it avoids numerical integrations throughout.

It is based on the modified minimal subtraction ($\overline{\rm MS}$) scheme which demonstrably avoids large expansion coefficients.

GAPP is endowed with the option to constrain non-standard contributions to the *oblique parameters* defined to affect only the gauge boson self-energies [2] (e.g. S, T, and U); specific anomalous Z couplings; the number of active neutrinos (with standard couplings to the Z boson); and the masses, mixings, and coupling strengths of extra Z bosons appearing in models of new physics. With view on the importance of supersymmetric extensions of the SM on one hand, and upcoming experiments on the other, I also included the $b \rightarrow s\gamma$ transition amplitude, and intend to add the muon anomalous magnetic moment. In the latter case, there are theoretical uncertainties from hadronic contributions which are partially correlated with the renormalization group (RG) evolutions of the QED coupling and the weak mixing angle. These correlations will be partially taken into account by including heavy quark effects in analytical form; see Ref. [3] for a first step in this direction. By comparing this scheme with more conventional ones, it will also be possible to isolate a QCD sum rule and to rigorously determine the charm and bottom quark $\overline{\rm MS}$ masses, $\hat{m}_c$ and $\hat{m}_b$, with high precision.

2. GAPP

2.1. Basic structure

In the default running mode of the current version, GAPP_99.7, a fit is performed to 41 observables, out of which 26 are from Z pole measurements at LEP 1 and the SLC. The Fermi constant, G_F (from the muon lifetime), the electromagnetic fine structure constant, α (from the quantum Hall effect), and the light fermion masses are treated as fixed inputs. The exception is

$\hat{m}_c$ which strongly affects the RG running[1] of $\hat{\alpha}(\mu)$ for $\mu > \hat{m}_c$. I therefore treat $\hat{m}_c$ as a fit parameter and include an external constraint with an enhanced error to absorb hadronic threshold uncertainties of other quark flavors, as well as theoretical uncertainties from the application of perturbative QCD at relatively low energies. Other fit parameters are the Z boson mass, M_Z, the Higgs boson mass, M_H, the top quark mass, m_t, and the strong coupling constant, α_s, so that there are 37 effective degrees of freedom. Given current precisions, M_Z may alternatively be treated as an additional fixed input.

The file `fit.f` basically contains a simple call to the minimization program MINUIT [4] (from the CERN program library) which is currently used in data driven mode (see `smfit.dat`). It in turn calls the core subroutine `fcn` and the χ^2-function `chi2`, both contained in `chi2.f`. Subroutine `fcn` defines constants and flags; initializes parts of the one-loop package FF [5, 6]; and makes the final call to subroutine `values` in `main.f` which drives the output (written to file `smfit.out`). In `chi2` the user actively changes and updates the data for the central values, errors, and correlation coefficients of the observables, and includes or excludes individual contributions to χ^2 (right after the initialization, `chi2 = 0.d0`). To each observable (as defined at the beginning of `chi2`) corresponds an entry in each of the fields `value, error, smval`, and `pull`, containing the central observed value, the total (experimental and theoretical) error, the calculated fit value, and the standard deviation, respectively. The function `chi2` also contains calls to various other subroutines where the actual observable calculations take place. These are detailed in the following subsections.

Another entry to GAPP is provided through `mh.f` which computes the probability distribution function of M_H. The probability distribution function is the quantity of interest within Bayesian data analysis (as opposed to point estimates frequently used in the context of classical methods), and defined as the product of a prior density and the likelihood, $\mathcal{L} \sim \exp(-\chi^2/2)$. If one chooses to disregard any further information on M_H (such as from triviality considerations or direct searches) one needs a *non-informative prior*. It is recommended to choose a flat prior in a variable defined on the whole real axis, which in the case of M_H is achieved by an equidistant scan over $\log M_H$. An *informative prior* is obtained by activating one of the approximate Higgs exclusion curves from LEP 2 near the end of `chi2.f`. These curves affect values of M_H even larger than the corresponding quoted 95% CL lower limit and includes an extrapolation to the

kinematic limit; notice that this corresponds to a conservative treatment of the upper M_H limit.

Contour plots can be obtained using the routine `mncontours` from MINUIT. For the cases this fails, some simpler and slower but more robust contour programs are also included in GAPP, but these have to be adapted by the user to the case at hand.

2.2. $\hat{\alpha}$, $\sin^2 \hat{\theta}_W$, M_W

At the core of present day electroweak analyses is the interdependence between G_F, M_Z, the W boson mass, M_W, and the weak mixing angle, $\sin^2 \theta_W$. In the $\overline{\text{MS}}$ scheme it can be written as [7, 8],

$$\hat{s}^2 = \frac{A^2}{M_W^2(1 - \Delta \hat{r}_W)}, \qquad \hat{s}^2 \hat{c}^2 = \frac{A^2}{M_Z^2(1 - \Delta \hat{r}_Z)}, \qquad (1)$$

where,

$$A = \left[\frac{\pi \alpha}{\sqrt{2} G_F} \right]^{1/2} = 37.2805(2) \text{ GeV}, \qquad (2)$$

$\hat{s}^2$ is the $\overline{\text{MS}}$ mixing angle, $\hat{c}^2 = 1 - \hat{s}^2$, and where,

$$\Delta \hat{r}_W = \frac{\alpha}{\pi} \hat{\Delta}_\gamma + \frac{\hat{\Pi}_{WW}(M_W^2) - \hat{\Pi}_{WW}(0)}{M_W^2} + \text{V} + \text{B}, \quad (3)$$

and,

$$\Delta \hat{r}_Z = \Delta \hat{r}_W + (1 - \Delta \hat{r}_W) \frac{\hat{\Pi}_{ZZ}(M_Z^2) - \frac{\hat{\Pi}_{WW}(M_W^2)}{\hat{c}^2}}{M_Z^2}, \quad (4)$$

collect the radiative corrections computed in `sin2th.f`. The $\hat{\Pi}$ indicate $\overline{\text{MS}}$ subtracted self-energies, and V + B denote the vertex and box contributions to μ decay. Although these relations involve the $\overline{\text{MS}}$ gauge couplings they employ on-shell gauge boson masses, absorbing a large class of radiative corrections [9].

$\Delta \hat{r}_W$ and $\Delta \hat{r}_Z$ are both dominated by the contribution $\hat{\Delta}_\gamma(M_Z)$ which is familiar from the RG running of the electromagnetic coupling,

$$\hat{\alpha}(\mu) = \frac{\alpha}{1 - \frac{\alpha}{\pi} \hat{\Delta}_\gamma(\mu)}, \qquad (5)$$

and computed in `alfahat.f` up to four-loop $\mathcal{O}(\alpha \alpha_s^3)$. Contributions from c and b quarks are calculated using an unsubtracted dispersion relation [3]. If μ is equal to the mass of a quark, three-loop matching is performed and the definition of $\hat{\alpha}$ changes accordingly. Pure QED effects are included up to next-to-leading order (NLO) while higher orders are negligible. Precise results can be obtained for $\mu < 2m_\pi$ and $\mu \geq m_c$.

Besides full one-loop electroweak corrections, $\Delta \hat{r}_W$ and $\Delta \hat{r}_Z$ include enhanced two-loop contributions of $\mathcal{O}(\alpha^2 m_t^4)$ [10] (implemented using the analytic expressions of Ref. [11]) and $\mathcal{O}(\alpha^2 m_t^2)$ [12]

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[1] Quantities defined in the $\overline{\text{MS}}$ scheme are denoted by a caret.

(available as expansions in small and large M_H); mixed electroweak/QCD corrections of $\mathcal{O}(\alpha\alpha_s)$ [13] and $\mathcal{O}(\alpha\alpha_s^2 m_t^2)$ [14]; the analogous mixed electroweak/QED corrections of $\mathcal{O}(\alpha^2)$; and fermion mass corrections also including the leading gluonic and photonic corrections.

2.3. Z decay widths and asymmetries

The partial width for $Z \to f\bar{f}$ decays is given by,

$$\Gamma_{f\bar{f}} = \frac{N_C^f M_Z \hat{\alpha}}{24\hat{s}^2\hat{c}^2} |\hat{\rho}_f| \left[1 - 4|Q_f|\mathrm{Re}(\hat{\kappa}_f)\hat{s}^2 + 8Q_f^2\hat{s}^4|\hat{\kappa}_f|^2\right]$$

$$\times \left[1 + \delta_{\mathrm{QED}} + \delta_{\mathrm{QCD}}^{\mathrm{NS}} + \delta_{\mathrm{QCD}}^{\mathrm{S}} - \frac{\hat{\alpha}\hat{\alpha}_s}{4\pi^2}Q_f^2 + \mathcal{O}(m_f^2)\right]. (6)$$

N_C^f is the color factor, Q_f is the fermion charge, and $\hat{\rho}_f$ and $\hat{\kappa}_f$ are form factors which differ from unity through one-loop electroweak corrections [15] and are computed in rho.f and kappa.f, respectively. For $f \neq b$ there are no corrections of $\mathcal{O}(\alpha^2 m_t^4)$ and contributions of $\mathcal{O}(\alpha^2 m_t^2)$ to $\hat{\kappa}_f$ [16] and $\hat{\rho}_f$ [9] are very small and presently neglected. On the other hand, vertex corrections of $\mathcal{O}(\alpha\alpha_s)$ [17] are important and shift the extracted α_s by ~ 0.0007.

The $Z \to b\bar{b}$ vertex receives extra corrections due to heavy top quark loops. They are large and have been implemented in bvertex.f based on Ref. [18]. $\mathcal{O}(\alpha^2 m_t^4)$ corrections [10, 11] are included, as well, while those of $\mathcal{O}(\alpha^2 m_t^2)$ are presently unknown. The leading QCD effects of $\mathcal{O}(\alpha\alpha_s m_t^2)$ [19] and all subleading $\mathcal{O}(\alpha\alpha_s)$ corrections [20] are incorporated into $\hat{\rho}_b$ and $\hat{\kappa}_b$, but not the $\mathcal{O}(\alpha\alpha_s^2 m_t^2)$ contribution which is presently available only for nonsinglet diagrams [21].

In Eq. (6), δ_{QED} are the $\mathcal{O}(\alpha)$ and $\mathcal{O}(\alpha^2)$ QED corrections. $\delta_{\mathrm{QCD}}^{\mathrm{NS}}$ are the universal QCD corrections up to $\mathcal{O}(\alpha_s^3)$ which include quark mass dependent contributions due to double-bubble type diagrams [22, 23]. $\delta_{\mathrm{QCD}}^{\mathrm{S}}$ are the singlet contributions to the axial-vector and vector partial widths which start, respectively, at $\mathcal{O}(\alpha_s^2)$ and $\mathcal{O}(\alpha_s^3)$, and induce relatively large family universal but flavor non-universal m_t effects [23, 24]. The corrections appearing in the second line of Eq. (6) are evaluated in lep100.f.

The dominant massless contribution to $\delta_{\mathrm{QCD}}^{\mathrm{NS}}$ can be obtained by analytical continuation of the Adler D-function, which (in the $\overline{\mathrm{MS}}$ scheme) has a very well behaved perturbative expansion $\sim 1 + \sum_{i=0} d_i a_s^{i+1}$ in $a_s = \hat{\alpha}_s(M_Z)/\pi$ (see the Appendix for details). The process of analytical continuation from the Euclidean to the physical region induces further terms which are proportional to β-function coefficients, enhanced by powers of π^2, and start at $\mathcal{O}(\alpha_s^3)$. Fortunately, these terms [25] involve only known coefficients up to $\mathcal{O}(\alpha_s^5)$, and the only unknown coefficient in $\mathcal{O}(\alpha_s^6)$ is proportional to the four-loop Adler function coefficient, d_3. In the massless approximation,

$$\delta_{\mathrm{QCD}}^{\mathrm{NS}} \approx a_s + 1.4092a_s^2 - (0.681 + 12.086)a_s^3 + \quad (7)$$

$$(d_3 - 89.19)a_s^4 + (d_4 + 79.7)a_s^5 + (d_5 - 121d_3 + 3316)a_s^6,$$

and terms of order $a_s^7 \sim 10^{-10}$ are clearly negligible. Notice, that the $\mathcal{O}(\alpha_s^6)$ term effectively *reduces* the sensitivity to d_3 by about 18%. Eq. (7) amounts to a reorganization of the perturbative series in terms of the d_i times some function of α_s; a similar idea is routinely applied to the perturbative QCD contribution to τ decays [26].

Final state fermion mass effects [22, 27] of $\mathcal{O}(m_f^2)$ (and $\mathcal{O}(m_b^4)$ for b quarks) are best evaluated by expanding in $\hat{m}_q^2(M_Z)$ thus avoiding large logarithms in the quark masses. The singlet contribution of $\mathcal{O}(\alpha_s^2 m_b^2)$ is also included.

The dominant theoretical uncertainty in the Z line-shape determination of α_s originates from the massless quark contribution, and amounts to about ± 0.0004 as estimated in the Appendix. There are several further uncertainties, all of $\mathcal{O}(10^{-4})$: from the $\mathcal{O}(\alpha_s^4)$ heavy top quark contribution to the axial-vector part of $\delta_{\mathrm{QCD}}^{\mathrm{S}}$; from the missing $\mathcal{O}(\alpha\alpha_s^2 m_t^2)$ and $\mathcal{O}(\alpha^2 m_t^2)$ contributions to the $Zb\bar{b}$-vertex; from further non-enhanced but cohering $\mathcal{O}(\alpha\alpha_s^2)$-vertex corrections; and from possible contributions of non-perturbative origin. The total theory uncertainty is therefore,

$$\Delta\alpha_s(M_Z) = \pm 0.0005, \quad (8)$$

which can be neglected compared to the current experimental error. If $\hat{m}_b$ is kept fixed in a fit, then its parametric error would add an uncertainty of ± 0.0002, but this would not change the total uncertainty (8).

Polarization asymmetries are (in some cases up to a trivial factor 3/4 or a sign) given by the asymmetry parameters,

$$A_f = \frac{1 - 4|Q_f|\mathrm{Re}(\hat{\kappa}_f)\hat{s}^2}{1 - 4|Q_f|\mathrm{Re}(\hat{\kappa}_f)\hat{s}^2 + 8Q_f^2\hat{s}^4|\hat{\kappa}_f|^2}, \quad (9)$$

and the forward-backward asymmetries by,

$$A_{FB}(f) = \frac{3}{4}A_e A_f. \quad (10)$$

The hadronic charge asymmetry, Q_{FB}, is the linear combination,

$$Q_{FB} = \sum_{q=d,s,b} R_q A_{FB}(q) - \sum_{q=u,c} R_q A_{FB}(q), \quad (11)$$

and the hadronic peak cross section, σ_{had}, is stored in sigmah, and defined by,

$$\sigma_{\mathrm{had}} = \frac{12\pi\Gamma_{e^+e^-}\Gamma_{\mathrm{had}}}{M_Z^2\Gamma_Z^2}. \quad (12)$$

Widths and asymmetries are stored in the fields `gamma(f)`, `alr(f)`, and `afb(f)`. The fermion index, `f`, and the partial width ratios, `R(f)`, are defined in Table 1.

Table 1

Some of the variables used in `lep100.f`. Γ_{inv} and Γ_{had} are the invisible and hadronic decays widths, respectively.

0	ν	`gamma(0)` $= \Gamma_{\text{inv}}$	`alr(0)` $= 1$
1	e	`R(1)` $= \Gamma_{\text{had}}/\Gamma_{e^+e^-}$	`alr(1)` $= A_e$
2	μ	`R(2)` $= \Gamma_{\text{had}}/\Gamma_{\mu^+\mu^-}$	`alr(2)` $= A_\mu$
3	τ	`R(3)` $= \Gamma_{\text{had}}/\Gamma_{\tau^+\tau^-}$	`alr(3)` $= A_\tau$
4	u	`R(4)` $= \Gamma_{u\bar{u}}/\Gamma_{\text{had}}$	—
5	c	`R(5)` $= \Gamma_{c\bar{c}}/\Gamma_{\text{had}}$	`alr(5)` $= A_c$
6	t	`R(6)` $= 0$	—
7	d	`R(7)` $= \Gamma_{d\bar{d}}/\Gamma_{\text{had}}$	—
8	s	`R(8)` $= \Gamma_{s\bar{s}}/\Gamma_{\text{had}}$	`alr(8)` $= A_s$
9	b	`R(9)` $= \Gamma_{b\bar{b}}/\Gamma_{\text{had}}$	`alr(9)` $= A_b$
10	had	`gamma(10)` $= \Gamma_{\text{had}}$	`afb(10)` $= Q_{FB}$
11	all	`gamma(11)` $= \Gamma_Z$	—

2.4. Fermion masses

I use $\overline{\text{MS}}$ masses as far as QCD is concerned, but retain on-shell masses for QED since renormalon effects are unimportant in this case. This results in a hybrid definition for quarks. Accordingly, the RG running of the masses to scales $\mu \neq \hat{m}_q$ uses pure QCD anomalous dimensions. The running masses correspond to the functions `msrun(`μ`)`, `mcrun(`μ`)`, etc. which are calculated in `masses.f` to three-loop order. Anomalous dimensions are also available at four-loop order [28], but can safely be neglected. Also needed is the RG evolution of α_s which is implemented to four-loop precision [29] in `alfas.f`.

I avoid pole masses for the five light quarks throughout. Due to renormalon effects, these can be determined only up to $\mathcal{O}(\Lambda_{\text{QCD}})$ and would therefore induce an irreducible uncertainty of about 0.5 GeV. In fact, perturbative expansions involving the pole mass show unsatisfactory convergence. In contrast, the $\overline{\text{MS}}$ mass is a short distance mass which can, in principle, be determined to arbitrary precision, and perturbative expansions are well behaved with coefficients of order unity (times group theoretical factors which grow only geometrically). Note, however, that the coefficients of expansions involving large powers of the mass, $\hat{m}^n$, are rather expected to be of $\mathcal{O}(n)$. This applies, e.g., to decays of heavy quarks ($n = 5$) and to higher orders in light quark mass expansions.

The top quark pole mass enters the analysis when the results on m_t from on-shell produced top quarks at the Tevatron are included. In subroutine `polemasses(nf,mpole)` $\hat{m}_q(\hat{m}_q)$ is converted to the quark pole mass, `mpole`, using the two-loop perturbative relation from Ref. [30]. The exact three-loop result [31] has been approximated (for m_t) by employing the BLM [32] scale for the conversion. Since the pole mass is involved it is not surprising that the coefficients are growing rapidly. The third order contribution is 31%, 75%, and 145% of the second order for m_t (`nf = 6`), m_b (`nf = 5`), and m_c (`nf = 4`), respectively. I take the three-loop contribution to the top quark pole mass of about 0.5 GeV as the theoretical uncertainty, but this is currently negligible relative to the experimental error. At a high energy lepton collider it will be possible to extract the $\overline{\text{MS}}$ top quark mass directly and to abandon quark pole masses altogether.

2.5. ν scattering

The ratios of neutral-to-charged current cross sections,

$$R_\nu = \frac{\sigma_{\nu N}^{NC}}{\sigma_{\nu N}^{CC}}, \qquad R_{\bar{\nu}} = \frac{\sigma_{\bar{\nu} N}^{NC}}{\sigma_{\bar{\nu} N}^{CC}}, \tag{13}$$

have been measured precisely in deep inelastic ν ($\bar{\nu}$) hadron scattering (DIS) at CERN (CDHS and CHARM) and Fermilab (CCFR). The most precise result was obtained by the NuTeV Collaboration at Fermilab who determined the Paschos-Wolfenstein ratio,

$$R^- = \frac{\sigma_{\nu N}^{NC} - \sigma_{\bar{\nu} N}^{NC}}{\sigma_{\nu N}^{CC} - \sigma_{\bar{\nu} N}^{CC}} \sim R_\nu - r R_{\bar{\nu}}, \tag{14}$$

with $r = \sigma_{\bar{\nu} N}^{CC}/\sigma_{\nu N}^{CC}$. Results on R_ν are frequently quoted in terms of the on-shell weak mixing angle (or M_W) as this incidentally gives a fair description of the dependences on m_t and M_H. One can write approximately,

$$R_\nu = g_L^2 + g_R^2 r, \quad R_{\bar{\nu}} = g_L^2 + \frac{g_R^2}{r}, \quad R^- = g_L^2 - g_R^2, \tag{15}$$

where,

$$g_L^2 = \frac{1}{2} - \sin^2\theta_W + \frac{5}{9}\sin^4\theta_W, \quad g_R^2 = \frac{5}{9}\sin^4\theta_W. \tag{16}$$

However, the study of new physics requires the implementation of the actual linear combinations of effective four-Fermi operator coefficients, $\epsilon_{L,R}(u)$ and $\epsilon_{L,R}(d)$, which have been measured. With the appropriate value for the average momentum transfer, `q2`, as input, these are computed in the subroutines `nuh(q2,epsu_L,epsd_L,epsu_R,epsd_R)` (according to Ref. [33]), `nuhnutev`, `nuhccfr`, and `nuhcdhs`, all contained in file `dis.f`. Note, that the

CHARM results have been adjusted to CDHS conditions [34]. While the experimental correlations between the various DIS experiments are believed to be negligible, large correlations are introduced by the physics model through charm mass threshold effects, quark sea effects, radiative corrections, etc. I constructed the matrix of correlation coefficients using the analysis in Ref. [34],

$$
\begin{array}{ccccccc}
R^- & R_\nu & R_\nu & R_\nu & R_{\bar\nu} & R_{\bar\nu} & R_{\bar\nu}
\end{array}
$$

$$
\begin{pmatrix}
1.00 & 0.10 & 0.10 & 0.10 & 0.00 & 0.00 & 0.00 \\
0.10 & 1.00 & 0.40 & 0.40 & 0.10 & 0.10 & 0.10 \\
0.10 & 0.40 & 1.00 & 0.40 & 0.10 & 0.10 & 0.10 \\
0.10 & 0.40 & 0.40 & 1.00 & 0.10 & 0.10 & 0.10 \\
0.00 & 0.10 & 0.10 & 0.10 & 1.00 & 0.15 & 0.15 \\
0.00 & 0.10 & 0.10 & 0.10 & 0.15 & 1.00 & 0.15 \\
0.00 & 0.10 & 0.10 & 0.10 & 0.15 & 0.15 & 1.00
\end{pmatrix} . (17)
$$

The effective vector and axial-vector couplings, $g_V^{\nu e}$ and $g_A^{\nu e}$, from elastic νe scattering are calculated in subroutine `nue(q2,gvnue,ganue)` in file `nue.f`. The momentum transfer, `q2`, is currently set to zero [36]. Needed is the low energy ρ parameter, `rhonc`, which describes radiative corrections to the neutral-to-charged current interaction strengths. Together with `sin2t0` (described below) it is computed in file `lowenergy.f`.

2.6. Low energy observables

The weak atomic charge, `Qw`, from atomic parity violation and fixed target ep scattering is computed in subroutine `apv(Qw,Z,AA,C1u,C1d,C2u,C2d)` where `Z` and `AA` are, respectively, the atomic number and weight. Also returned are the coefficients from lepton-quark effective four-Fermi interactions which are calculated according to [37].

These observables are sensitive to the low energy mixing angle, `sin2t0`, which defines the electroweak counterpart to the fine structure constant and is similar to the one introduced in Ref. [7]. There is significant correlation between the hadronic uncertainties from the RG evolutions of $\hat\alpha$ and the weak mixing angle. Presently, this correlation is ignored, but with the recent progress in atomic parity violation experiments it should be accounted for in the future.

An additional source of hadronic uncertainty is introduced by γZ-box diagrams which are unsuppressed at low energies. At present, this uncertainty can be neglected relative to the experimental precision.

Besides `apv`, file `pnc.f` contains in addition the subroutine `moller` for the anticipated polarized fixed target Møller scattering experiment at SLAC. Radiative corrections are included following Ref. [38].

2.7. $b \to s\gamma$

Subroutine `bsgamma` returns the decay ratio,

$$
R = \frac{\mathcal{B}(b \to s\gamma)}{\mathcal{B}(b \to ce\nu)}. \tag{18}
$$

It is given by [39, 40],

$$
R = \frac{6\alpha}{\pi} \left| \frac{V_{ts}^* V_{tb}}{V_{cb}} \right|^2 \frac{S}{f(z)} \frac{|\bar{D}|^2 + A/S + \delta_{NP} + \delta_{EW}}{(1+\delta_{NP}^{SL})(1+\delta_{EW}^{SL})}, (19)
$$

where $|V_{ts}^* V_{tb}/V_{cb}|^2 = 0.950$ is a combination of Cabbibo-Kobayashi-Maskawa matrix elements and S is the Sudakov factor [41]. δ_{NP} and δ_{EW} are nonperturbative and NLO electroweak [42] corrections, both for the $b \to s\gamma$ and the semileptonic ($b \to ce\nu$) decay rates.

$$
\bar{D} = C_7^0 + \frac{\hat\alpha_s(\hat m_b)}{4\pi}(C_7^1 + V), \tag{20}
$$

is called the reduced amplitude for the process $b \to s\gamma$, and is given in terms of the Wilson coefficient C_7 at NLO. C_7 and the other C_i appearing below are effective Wilson coefficients with NLO RG evolution [43] from the weak scale to $\mu = \hat m_b$ understood. The NLO matching conditions at the weak scale have been calculated in Ref. [44]. $\bar{D}$ includes the virtual gluon corrections,

$$
V = r_2 C_2^0 + r_7 C_7^0 + r_8 C_8^0, \tag{21}
$$

so that it squares to a positive definite branching fraction. On the other hand, the amplitude for gluon Bremsstrahlung ($b \to s\gamma g$),

$$
A = \frac{\hat\alpha_s(\hat m_b)}{\pi}[C_2^0(C_8^0 f_{28}(1) + C_7^0 f_{27}(1) + C_2^0 f_{22}(1))+
$$

$$
C_8^0(C_8^0 f_{88}(\delta) + C_7^0 f_{78}(\delta)) + (C_7^0)^2 f_{77}(\delta)], \tag{22}
$$

is added linearly to the cross section. The Wilson coefficient C_2^0 is defined as in Ref. [45]. It enters only at NLO, is significantly larger than C_7^0, and dominates the NLO contributions. The parameter $0 \le \delta \le 1$ in the coefficient functions f_{ij} characterizes the minimum photon energy and has been set to $\delta = 0.9$ [41], except for the first line in Eq. (22) where $\delta = 1.0$ corresponding to the full cross section. The f_{2i} are complicated integrals which can be solved in terms of polylogarithms up to 5th order. In the code I use an expansion in $z = m_c^2/m_b^2$ and $\delta = 1.0$. Once experiments become more precise the correction to $\delta = 0.9$ should be included.

$f(z)$ is the phase space factor for the semileptonic decay rate including NLO corrections [46]. I defined the $\overline{\text{MS}}$ mass ratio in $z = [\hat m_c(\hat m_b)/\hat m_b(\hat m_b)]^2$ at the common scale, $\mu = \hat m_b$, which I also assumed for the factor $\hat m_b^5$ multiplying the decay widths. Since I do not

reexpand the denominator this effects the phase space function at higher orders. Using the $\mathcal{O}(\alpha_s^2)$-estimate[2] from Ref. [47], I obtain for the semileptonic decay width,

$$\Gamma_{SL} \sim \hat{m}_b^5 f_0(z) \left[1 + 2.7 \frac{\hat{\alpha}_s(\hat{m}_b)}{\pi} - 1.6 \left(\frac{\hat{\alpha}_s}{\pi} \right)^2 \right], \quad (23)$$

where $f_0(z)$ is the leading order phase space factor. It is amusing that the coefficients in Eq. (23) are comfortably (and perhaps somewhat fortuitously) small, with the $\mathcal{O}(a_s^2)$-coefficient even smaller than the one in Ref. [47] where a low scale running mass had been advocated. Moreover, using the prefactor $\hat{m}_b^5$ in the numerator of R reduces the size of r_7 in Eq. (21) and therefore the coefficient $\kappa(\delta) = f_{77}(\delta) + r_7/2$ which multiplies the term $a_s(C_7^{0,\text{eff}})^2$. I obtain $-2.1 < \kappa(\delta) < 1.4$, while with the pole mass prefactor M_b^5 one would have $-8.7 \leq \kappa(\delta) < -5.3$.

Acknowledgements

A. Uncertainties from perturbative QCD

Writing the perturbative expansion of some quantity in its general form for an arbitrary gauge group, it can easily be decomposed into separately gauge invariant parts. Table 2 shows for some (related) examples that after removing the group theoretical prefactors, all coefficients, y_i, are *strictly* of order unity, and that their mean, $\bar{y}$, is very close to zero. In particular, there is no sign of factorial growth of coefficients. These observations offer a valuable tool to estimate the uncertainties associated with the truncation of the loop expansion, so I would like to make them more precise.

Assume (for simplicity) that the y_i are random draws from some normal distribution with unknown mean, μ, and variance, σ^2. One can show that the marginal distribution of μ follows a Student-t distribution with $n - 1$ degrees of freedom, t_{n-1}, centered about $\bar{y}$, and with standard deviation,

$$\Delta\mu = \sqrt{\frac{\sum_i (y_i - \bar{y})^2}{n(n-3)}}. \quad (24)$$

As can be seen from the Table, μ is consistent with zero in all cases, justifying the nullification of the unknown coefficients from higher loops. I next assert that the

[2]I computed the $\mathcal{O}(\alpha_s^2)$ coefficient for comparison only, and did not include it in the code.

distribution of σ, conditional on $\mu = 0$, follows a scaled inverse-χ^2 distribution with n degrees of freedom, from which I obtain the estimate,

$$\sigma = \sigma_0 \pm \Delta\sigma = \sqrt{\frac{\sum_i y_i^2}{n-2}} \left[1 \pm \sqrt{\frac{1}{2(n-4)}} \right]. \quad (25)$$

Inspection of the Table shows indeed that σ, as the typical size of a coefficient, is estimated to be $\lesssim \mathcal{O}(1)$.

I now focus on the partial hadronic Z decay width. As discussed in Section 2.3, the $\mathcal{O}(\alpha_s^3)$ term, d_2, is much smaller than the π^2 term arising from analytical continuation. This is specifically true for the relevant case of $n_f = 5$ active flavors, where large cancellations occur between gluonic and fermionic loops. Notice, that the D-function, in contrast to R_{had}, has opposite signs in the leading terms proportional to $C_A^2 C_F$ and $C_A C_F T_F n_F$. Indeed, the Adler D-function and the β-function have similar structures regarding the signs and sizes of the various terms (see Table 2), and we *do expect* large cancellations in the β-function. The reason is that it has to vanish identically in the case of $N = 4$ supersymmetry. Ignoring scalar contributions this case can be mimicked by setting $T_F n_f = 2C_A$ (there are 2 Dirac fermions in the $N = 4$ gauge multiplet) or $n_f = 12$ for QCD, which is of the right order. In fact, all known QCD β-function coefficients become very small for some value of n_f between 6 and 16. We therefore have a reason to expect that similar cancellations will reoccur in the d_i at higher orders. As a 1σ error estimate for d_3, I suggest to use the largest known coefficient (3×0.71) times the largest group theoretical prefactor in the next order $(C_A^3 C_F)$ which results in

$$d_3 = 0 \pm 77. \quad (26)$$

With Eq. (7) and $\hat{\alpha}_s(M_Z) = 0.120$ one can absorb all higher order effects into the $\mathcal{O}(\alpha_s^4)$-coefficient of R_{had}, $r_3^{\text{eff}} = -81 \pm 63$. This shifts the extracted α_s from the Z lineshape by $+0.0005$ and introduces the small uncertainty of ± 0.0004.

The argument given above does certainly not apply to the *quenched* case, $n_f = 0$, and indeed $d_2(n_f = 0)$ is about -73% of the π^2 term, i.e., large and positive. In the case of $n_f = 3$, which is of interest for the precision determination of α_s from τ decays, d_2 is about -38% of the π^2 term. If one assumes that the same is true of d_3, one would obtain $d_3(n_f = 3) = 60$. Estimates based on the principles of minimal sensitivity, PMS, or fastest apparent convergence, FAC, yield $d_3(n_f = 3) = 27.5$ [25] so there might be some indications for a positive $d_3(n_f = 3)$. In any case, all these estimates lie within the uncertainty in Eq. (26) and we will have to await the proper calculation of the $\mathcal{O}(\alpha_s^4)$-coefficient to test these hypotheses. Note, that the current τ decay

analysis by the ALEPH Collaboration uses $d_3 = 50 \pm 50$ [50] which is more optimistic.

The analogous error estimate for the five-loop β-function coefficient yields,

$$\beta_4 = 0 \pm 579. \tag{27}$$

To get an estimate for the uncertainty in the RG running of $\hat{\alpha}_s$, I translate Eq. (27) into

$$\beta_3 = \beta_3 \pm \frac{\hat{\alpha}_s(\mu_0)}{\pi}\beta_4, \tag{28}$$

where μ_0 is taken to be the lowest scale involved. This overestimates the uncertainty from β_4, thereby compensating for other neglected terms of $\mathcal{O}(\alpha_s^{n+4}\ln^n\mu^2/\mu_0^2)$. For the RG evolution from $\mu = m_\tau$ to $\mu = M_Z$ this yields an uncertainty of $\Delta\alpha_s(M_Z) = \pm 0.0005$. Conversely, for fixed $\alpha_s(M_Z) = 0.120$, I obtain $\hat{\alpha}_s(\hat{m}_b) = 0.2313 \pm 0.0006$, $\hat{\alpha}_s(m_\tau) = 0.3355 \pm 0.0045$, and $\hat{\alpha}_s(\hat{m}_c) = 0.403 \pm 0.011$, where I have used $\hat{m}_b = 4.24$ GeV and $\hat{m}_c = 1.31$ GeV. For comparison, the ALEPH Collaboration quotes an evolution error of $\Delta\alpha_s(M_Z) = \pm 0.0010$ which is twice as large. I emphasize that it is important to adhere to consistent standards when errors are estimated. This is especially true in the context of a global analysis where the precisions of the observables enter as their relative weights.

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Table 2

Coefficients ($\overline{\text{MS}}$) appearing in the β-function of a simple group [29]; in non-Abelian corrections to the QED β-function (denoted $\tilde{D}$) [3, 48]; in the Adler D-function [49] (rescaled by an overall factor 1/3); and in R_{had} (analytical continuation of D). The first four segments correspond, respectively, to the first four loop orders of non-singlet type. The fifth segment is the singlet (double triangle) contribution in $\mathcal{O}(\alpha_s^3)$. In $\tilde{D}$, D, and R_{had}, an overall factor $\hat{\alpha}M_Z$ and the sums involving charges or Z couplings have been dropped. The completely symmetrical tensors of rank four, d_A and d_F, as well as T_F when appearing in parenthesis, apply to the β-function only. Each T_F is understood to be multiplied by the number of flavors, n_f, except for the singlet term involving the symmetrical structure constants, d.

group factor	β	$\tilde{D}$	D	R_{had}
C_A	0.92	—	—	—
(T_F)	-0.33	-0.33	0.33	0.33
C_A^2	0.71	—	—	—
$C_A T_F$	-0.42	—	—	—
$C_F(T_F)$	-0.25	-0.25	0.25	0.25
C_A^3	0.83	—	—	—
$C_A^2 T_F$	-0.82	—	—	—
$C_A C_F(T_F)$	-0.36	-0.23	0.18	0.18
$C_A T_F^2$	0.09	—	—	—
$C_F^2(T_F)$	0.03	0.03	-0.03	-0.03
$C_F T_F(T_F)$	0.08	0.08	-0.06	-0.06
C_A^4	1.19	—	—	—
$C_A^3 T_F$	-1.67	—	—	—
$C_A^2 C_F(T_F)$	-0.23	-0.28	0.32	-0.38
$C_A^2 T_F^2$	0.50	—	—	—
$C_A C_F^2(T_F)$	-0.42	-0.07	0.51	0.51
$C_A C_F T_F(T_F)$	0.51	0.42	-0.71	-0.21
$C_A T_F^3$	0.01	—	—	—
$C_F^3(T_F)$	0.18	0.18	-0.18	-0.18
$C_F^2 T_F(T_F)$	-0.17	-0.17	0.02	0.02
$C_F T_F^2(T_F)$	0.02	0.02	0.09	-0.01
d_A^2/N_A	1.07	—	—	—
$d_A d_F/N_A$	-2.38	—	—	—
d_F^2/N_A $(T_F^2 d^2/4)$	0.50	0.50	-0.50	-0.50
$\bar{y}$	-0.02	-0.01	0.02	-0.01
$\Delta\mu$	0.17	0.09	0.11	0.09
σ_0	0.83	0.28	0.37	0.31
$\Delta\sigma$	0.13	0.07	0.09	0.08