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APPLICATION OF PADE APPROXIMANTS TO DETERMINATION OF $\alpha_s(M_Z^2)$ FROM HADRONIC EVENT SHAPE OBSERVABLES IN e^+e^- ANNIHILATION*

P.N. Burrows
Massachusetts Institute of Technology
Cambridge, MA 02139, USA

T. Abraha, M. Samuel, E. Steinfelds
Department of Physics
Oklahoma State University
Stillwater, OK 74078, USA

H. Masuda
Stanford Linear Accelerator Center
Stanford University, Stanford, CA 94309, USA

ABSTRACT

We have applied Padé approximants to perturbative QCD calculations of event shape observables in $e^+e^- \rightarrow$ hadrons. We used the exact $O(\alpha_s^2)$ prediction and the [0/1] Padé approximant to estimate the $O(\alpha_s^3)$ term for 15 observables, and in each case determined $\alpha_s(M_Z^2)$ from comparison with hadronic Z^0 decay data from the SLD experiment. We found the scatter among the $\alpha_s(M_Z^2)$ values to be significantly reduced compared with the standard $O(\alpha_s^2)$ determination, implying that the Padé method provides at least a partial approximation of higher-order perturbative contributions to event shape observables.

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One of the most important tasks in high energy physics is the precise determination of the strong coupling α_s, conventionally expressed at the scale of the mass of the Z^0 boson, $M_Z \simeq 91.2$ GeV. Not only does measurement of $\alpha_s(M_Z^2)$ in different hard processes and at different hard scales Q provide a fundamental test of the theory of strong interactions, Quantum Chromodynamics (QCD), but it also allows constraints on extensions to the Standard Model of elementary particles. For example, it has been claimed [1] that measurements of electroweak observables can be better described by the Standard Model with $\alpha_s(M_Z^2) = 0.112$ and the addition of light superpartners, than by the Standard Model alone with $\alpha_s(M_Z^2) = 0.123$. The latter study, as well as studies of other possible extensions to the Standard Model [2], have been prompted by claims [3] that recent measurements of $\alpha_s(M_Z^2)$ may be grouped into two classes: those made at 'low-Q^2', which tend to cluster at values around 0.112, and those made at 'high-Q^2', which tend to cluster at values around 0.123; for a review of these measurements see Ref. [4].

Examination of the large set of $\alpha_s(M_Z^2)$ measurements reveals that in fact all are consistent with a 'world average' central value of about 0.117 with an uncertainty of ± 0.005 [4], and that their grouping into two supposedly discrepant classes is arbitrary and not significant. Furthermore, nearly all measurements are limited by theoretical systematic uncertainties that derive from lack of knowledge of higher-order perturbative QCD contributions, or of non-perturbative effects, or both. The effects on $\alpha_s(M_Z^2)$ determinations of such uncalculated contributions have been estimated using *ad hoc* procedures, sometimes in different ways by different experimental collaborations working in similar areas; see *eg.* [5,6]. It appears to us premature to speculate on beyond-Standard Model explanations of $\alpha_s(M_Z^2)$ measurements that, within large, dominant and arbitrarily-estimated theoretical uncertainties, are consistent with one another. We suggest that a more rational approach is to reduce the size of the limiting theoretical uncertainties which may, or may not, be concealing new physics.

Here we consider hadronic event shape observables in e^+e^- annihilation, for which perturbative QCD calculations have been performed exactly only up to second order in α_s [7,8] and have been used extensively by collaborations at the PETRA, PEP, TRISTAN, SLC, and LEP colliders for measurement of $\alpha_s(M_Z^2)$ [4]. A large scatter among the $\alpha_s(M_Z^2)$ values derived from different observables has been found [9,10], which can in principle be accounted for as an effect of the *a priori* unknown higher order contributions in perturbation theory. A consensus has arisen among experimentalists to estimate the size of this effect for each observable from the renormalisation-scale (μ) dependence of the $\alpha_s(M_Z^2)$ values derived from fits of the $O(\alpha_s^2)$ calculation to the data, see *eg.* [10], and to quote a corresponding renormalisation scale uncertainty on $\alpha_s(M_Z^2)$. Within such uncertainties the $\alpha_s(M_Z^2)$ values from the different observables are found to be consistent, but this (arbitrary) procedure naturally leads to a large uncertainty on the final $\alpha_s(M_Z^2)$ averaged over all observables; for example, using 15 observables the SLD Collaboration determined [10]:

$$\alpha_s(M_Z^2) \quad = \quad 0.1226 \pm 0.0025\,(\text{exp.}) \pm 0.0109\,(\text{theor.}) \tag{1}$$

where the theoretical uncertainty is dominated by the contribution of ± 0.0106 from the renormalisation scale variation.

The best resolution of this situation would be to calculate the observables to higher order in perturbation theory, a difficult and unattractive task that has not yet been achieved. In the absence of $O(\alpha_s^3)$ QCD calculations it has been suggested

[11,12,13] that the $O(\alpha_s^2)$ calculation for each observable can be 'optimised' by choosing a specific value of the renormalisation scale. It has recently been shown [6] that such optimised scale choices do not serve to reduce the scatter among the $\alpha_s(M_Z^2)$ values determined from different observables, which implies that they do not reduce the size of the contributions from the uncalculated higher orders.

Here we employ an approach for estimating the $O(\alpha_s^3)$ contributions to, as well as the sum of, the perturbative QCD series for event shape observables in e^+e^- annihilation. The method makes use of Padé Approximants (PA). The PA method has been applied to estimate coefficients in perturbative quantum field theory and statistical physics [14] and is outlined in detail in Ref. [15]. We give a brief review here.

The PA $[N/M]$ to the series:

$$S \quad = \quad S_0 \ + \ S_1 x \ + \ S_2 x^2 \ + \ \ldots \ + \ S_{N+M} x^{N+M} \tag{2}$$

is defined [16]:

$$[N/M] \quad \equiv \quad \frac{a_0 + a_1 x + a_2 x^2 + \ldots + a_N x^N}{1 + b_1 x + b_2 x^2 + \ldots + b_M x^M}, \tag{3}$$

where N and M are integers such that $N \geq 0$ and $M > 0$, and

$$[N/M] \quad = \quad S + O(x^{N+M+1}). \tag{4}$$

The coefficients a_i $(0 \leq i \leq N)$ and b_j $(1 \leq j \leq M)$ are obtained by multiplying Eq. 4 by the denominator of Eq. 3 and equating coefficients of like powers of x. By consideration of the terms of $O(x^{N+M+1})$ one can obtain an estimate of the coefficient S_{N+M+1}. Furthermore, for an asymptotic series $[N/M]$ can be taken to be an estimate of the sum of the series to all orders; we refer to this as the Padé sum (PS).

Recently this method has been applied to estimate the O(α_s^3) term in the perturbative QCD prediction for the inclusive quantities $R = \sigma(e^+e^- \rightarrow \text{hadrons})/\sigma(e^+e^- \rightarrow \mu^+\mu^-)$, $R_\tau = \Gamma(\tau\rightarrow \nu \text{ hadrons})/\ \Gamma(\tau\rightarrow e\overline{\nu}_e\nu_\tau)$ and the Bjorken sum rule in deep inelastic scattering [17]. In each case the PA estimate is in good agreement with the exact calculation of the O(α_s^3) term, which is remarkable since the method does not involve knowledge of strong interaction dynamics. Based upon this success PA estimates have also been made of O(α_s^4) terms for the same quantities [17,18].

In the case of e$^+$e$^-$ annihilation into hadronic final states the perturbative QCD prediction for an infra-red- and collinear-safe observable X can be written:

$$\frac{1}{\sigma}\frac{d\sigma}{dX}(X,\mu) = \overline{\alpha_s}(\mu)A(X) + \overline{\alpha_s}^2(\mu)\ B(X,\mu) + \overline{\alpha_s}^3(\mu)\ C(X,\mu) + O(\overline{\alpha_s}^4(\mu)) \qquad (5)$$

where $\overline{\alpha_s} \equiv \alpha_s/2\pi$. To date only the leading and next-to-leading coefficients $A(X)$ and $B(X,\mu)$ have been calculated [7,8]. Throughout this paper we set the renormalisation scale μ to the so-called physical value $\mu = Q = \sqrt{s}$; in this case the μ-dependence of the beyond-leading coefficients B, C, ... vanishes.

We have employed the 15 hadronic event shape observables used in the recent $\alpha_s(M_Z^2)$ determination by the SLD Collaboration [10], namely 1−thrust (τ), oblateness (O), the C-parameter (C), normalised heavy jet mass (ρ), total jet broadening (B_T), wide jet broadening (B_W), the differential 2-jet rate defined using the E, E0, P, P0, D and G algorithms (D_2^E, D_2^{E0}, D_2^P, D_2^{P0}, D_2^D and D_2^G respectively), energy-energy correlations (EEC) and their asymmetry ($AEEC$), and the Jet Cone Energy Fraction ($JCEF$) [19]. Distributions of these 15 event shape observables were measured [10] using a sample of approximately 50,000 hadronic Z^0 decay events. The data were corrected for detector bias effects such as acceptance, resolution, and inefficiency, as well as for the effects of initial-state radiation and hadronisation, to arrive at 'parton-level' distributions, which can be compared directly with the QCD calculations.

For each observable X we employed the EVENT program [20] to calculate the coefficients $A(X)$ and $B(X)$ in Eq. 5. These coefficients are listed in Table 1 for a representative value of each observable. In each case it can be seen that the next-to-leading coefficient B is typically an order of magnitude larger than the leading coefficient A. At first sight this appears to make the perturbative approach invalid; it should be noted, however, that the ratio of next-to-leading to leading terms in Eq. 5 contains an additional factor of $\overline{\alpha_s}$, which is about 1/52 for $\alpha_s(M_Z^2) = 0.12$, so that in all cases the next-to-leading term is smaller than the leading term.

By explicitly separating an overall factor of $\overline{\alpha_s}$ on the r.h.s. of Eq. 5 and comparing with the form of Eq. 2 the PA [0/1] can be defined for the series. For each bin of each observable, by consideration of the PA [0/1] we derived an estimate of the coefficient $C(X)$ of the next-to-next-to-leading term in the series:

$$C(X) \quad = \quad \frac{B(X)^2}{A(X)}. \tag{6}$$

Examples of the predictions for $C(X)$ are given in Table 1. It follows from Eq. 6 that $C(X) \geq 0$ and that the ratios $C(X)/B(X)$ and $B(X)/A(X)$ are equal. For each bin of each observable we added the PA prediction for the $\mathrm{O}(\alpha_s^3)$ term to the exact $\mathrm{O}(\alpha_s^2)$ calculation to obtain an estimate of the series to $\mathrm{O}(\alpha_s^3)$. For each observable we then fitted these calculations simultaneously to all bins in the selected range of the data [10] by minimising χ^2 w.r.t. variation of $\alpha_s(M_Z^2)$. The resulting $\alpha_s(M_Z^2)$ and χ^2_{dof} values are shown in Table 2.

It should be noted that the O(α_s^3) estimate does not provide a good fit to the B_T data, as indicated by the large χ^2_{dof} value (Table 2). It is perhaps significant that this observable shows a large renormalisation scale uncertainty on $\alpha_s(M_Z^2)$ determined at O(α_s^2) [10], and has a very large ratio of next-to-leading to leading order coefficients (Table 1), both implying that beyond-next-to-leading order contributions may be large. Furthermore, the latter suggests that the PA [0/1] estimate of the next-to-next-to-leading order coefficient may be neither reliable, nor sufficient to describe the data as is observed. In the following discussion we therefore exclude B_T and restrict the analysis to the remaining 14 observables; however, we indicate in footnotes to the text any relevant changes in results if B_T is included.

The $\alpha_s(M_Z^2)$ values are shown in Fig. 1, together with the corresponding values from the O(α_s^2) analysis of the SLD data with $\mu = \sqrt{s}$ [6]. For each observable it can be seen that the $\alpha_s(M_Z^2)$ value derived using the O(α_s^3) estimate is lower than that derived using the O(α_s^2) calculation, which is expected since $C(X)$ is positive. Also shown for each observable is the total uncertainty on $\alpha_s(M_Z^2)$ from the SLD O(α_s^2) study [10], which is dominated by the renormalisation scale variation. In each case the O(α_s^3) $\alpha_s(M_Z^2)$ value lies near the lower bound given by the scale uncertainty on the O(α_s^2) result. To the extent that the PA O(α_s^3) estimate is accurate, this implies that the uncertainty assigned to the O(α_s^2) $\alpha_s(M_Z^2)$ value from each observable due to variation of the renormalisation scale is a reasonable estimate of the effect of the missing O(α_s^3) contribution.

Furthermore, it can be seen from Fig. 1 that the scatter among the $\alpha_s(M_Z^2)$ values is noticeably smaller in the $\mathrm{O}(\alpha_s^3)$ case. Taking an unweighted average[1] and r.m.s. deviation over each set of 14 $\alpha_s(M_Z^2)$ values yields[2]:

$$\alpha_s(M_Z^2) \quad = \quad 0.1255 \pm 0.0070 \qquad (O(\alpha_s^2)) \tag{7}$$

$$\alpha_s(M_Z^2) \quad = \quad 0.1147 \pm 0.0035 \qquad (O(\alpha_s^3)), \tag{8}$$

implying that the inclusion of $\mathrm{O}(\alpha_s^3)$ terms causes a reduction in the central value of $\alpha_s(M_Z^2)$ at $\mu = \sqrt{s}$ by approximately 0.011, and that the residual scatter among the $\mathrm{O}(\alpha_s^3)$ $\alpha_s(M_Z^2)$ values, presumably due to missing $\mathrm{O}(\alpha_s^4)$ terms, is approximately ± 0.0035, which is comparable with the combined experimental error and hadronisation uncertainty on a single observable measured at $Q = M_Z$ [10]. Since the accuracy of the Padé Approximant method can only be verified *a posteriori*, exact calculation of the $\mathrm{O}(\alpha_s^3)$ terms in order to confirm these results would be extremely desirable.

We also used the PS [0/1] as an estimate of the sum of the asymptotic series and extracted $\alpha_s(M_Z^2)$ by comparison with the data in a similar manner. The $\alpha_s(M_Z^2)$ values are shown in Fig. 1. Typically, for each observable, the PS $\alpha_s(M_Z^2)$ value is close to the $\mathrm{O}(\alpha_s^3)$ value. Again the fit to B_T is very poor, and we omit it from the following main discussion. Taking an unweighted average and r.m.s. deviation over the set of 14 $\alpha_s(M_Z^2)$ values yields[3]:

$$\alpha_s(M_Z^2) \quad = \quad 0.1148 \pm 0.0052 \qquad (\mathrm{PS}). \tag{9}$$

[1] Weighted averages using experimental errors [10] yield mean $\alpha_s(M_Z^2)$ values consistent with the respective unweighted averages within the statistical error on a single $\alpha_s(M_Z^2)$ value.

[2] Including B_T and averaging over 15 observables yields $\alpha_s(M_Z^2) = 0.1265 \pm 0.0076$ ($\mathrm{O}(\alpha_s^2)$) and $\alpha_s(M_Z^2) = 0.1139 \pm 0.0045$ ($\mathrm{O}(\alpha_s^3)$).

[3] Including B_T and averaging over 15 observables yields $\alpha_s(M_Z^2) = 0.1136 \pm 0.0068$.

Though the average value is close to that obtained using the PA $O(\alpha_s^3)$ estimate, the r.m.s. deviation is somewhat larger, implying that the PS [0/1] provides a poorer estimate of the sum of the series than the PA [0/1] estimate to $O(\alpha_s^3)$.

Other interesting features are apparent from Fig. 1. Several observables yield noticeably larger scale uncertainty at $O(\alpha_s^2)$, namely τ, B_T, O, C, D_2^E and EEC, which is an indication of potentially large contributions at $O(\alpha_s^3)$ that is supported by the PA and PS [0/1] estimates. If these are omitted from consideration the remaining set of observables yields average and r.m.s. $\alpha_s(M_Z^2)$ values of 0.1212 ± 0.0044 ($O(\alpha_s^2)$ analysis), 0.1131 ± 0.0028 ($O(\alpha_s^3)$ analysis) and 0.1155 ± 0.0025 (PS analysis). Though the selection of this subset is arbitrary, it is perhaps noteworthy that both Padé-derived $\alpha_s(M_Z^2)$ values are close to the corresponding values [6] obtained with $O(\alpha_s^2)$ calculations and 'PMS' [11] and 'FAC' [12] optimised scales, 0.1146 ± 0.0025 and 0.1148 ± 0.0025 respectively, and that the scatter is similarly small[4].

In summary, we have applied Padé approximants to the determination of $\alpha_s(M_Z^2)$ from hadronic event shape observables in e^+e^- annihilation. We applied the PA [0/1] to the $O(\alpha_s^2)$ perturbative QCD series for 15 observables to obtain estimates of the $O(\alpha_s^3)$ coefficients, and then fitted the extended series to SLD data to determine $\alpha_s(M_Z^2)$. With the renormalisation scale fixed to the c.m. energy the scatter (neglecting B_T) among the $\alpha_s(M_Z^2)$ values was reduced from ± 0.0070 ($O(\alpha_s^2)$) to ± 0.0035 ($O(\alpha_s^3)$), and the central value of $\alpha_s(M_Z^2)$ was lowered by 0.011. If the scatter is interpreted as arising from missing higher-order contributions, the reduction in scatter implies that the Padé method provides at least a partial approximation of higher-order perturbative QCD contributions to event shape observables. Furthermore, if the Padé-estimated $O(\alpha_s^3)$ terms are accurate, this result

[4] Significantly larger scatter is obtained with the 'BLM' scale choice: $\alpha_s(M_Z^2) = 0.1082 \pm 0.0091$.

implies that residual $O(\alpha_s^4)$ terms contribute to $\alpha_s(M_Z^2)$ at the level of ± 0.0035, which is comparable with current experimental and hadronisation uncertainties.

These results based on Padé approximants are tantalising, but they can only be verified upon completion of a full perturbative QCD calculation at $O(\alpha_s^3)$, which we strongly encourage. One could then apply the [0/2] or [1/1] Padé approximants to the $O(\alpha_s^3)$ series in order to estimate the size of $O(\alpha_s^4)$ contributions. Since the accuracy of the Padé method in predicting unknown perturbation series coefficients is expected to improve with increasing order of the known terms, it can be argued that the estimated $O(\alpha_s^4)$ coefficients would be expected to be more accurate than the estimates of $O(\alpha_s^3)$ coefficients presented here[5]. Combined with recent theoretical progress in understanding hadronisation effects in terms of 'power corrections' [21], it may then be plausible to expect that $\alpha_s(M_Z^2)$ measurements at the 1%-level of precision could be achieved at future high-energy e^+e^- colliders [22].

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[5] See Refs. [17,18] for $O(\alpha_s^4)$ estimates for R, R_τ and the Bjorken sum rule.

REFERENCES

1. G.L. Kane *et al.*, Phys. Lett. **B354** (1995) 350.
2. M. Bastero-Gil, B. Brahmachari, Phys. Rev. **D54** (1996) 1063.

   B. Brahmachari, R. Mohapatra, Int. J. Mod. Phys. **A11** (1996) 1699.

   J. Ellis, J.L. Lopez, D.V. Nanopoulos, Phys. Lett. **B371** (1996) 65.

   J. K. Kim *et al.*, Phys. Rev. **D53** (1996) 1712.

   P.H. Frampton *et al.*, preprint HEP-PH/9511445 (1995).
3. See *eg.*: M. Shifman, Mod. Phys. Lett. **A10** No. 7 (1995) 605.
4. P.N. Burrows, SLAC-PUB-7293; to appear in Proc. Int. Symposium on Radiative Corrections, Cracow, 1996.
5. P.N. Burrows, H. Masuda, Z. Phys. **C63** (1994) 235.
6. P.N. Burrows *et al.*, Phys. Lett. **B382** (1996) 157.
7. R.K. Ellis, D.A. Ross, A.E. Terrano, Phys. Rev. Lett. **45** (1980) 1226; Nucl. Phys. **B178** (1981) 421.

   G. Kramer, B. Lampe, Z. Phys. **C39** (1988) 101; Fortschr. Phys. **37** (1989) 161.
8. Z. Kunszt *et al.*, CERN 89–08 Vol I, (1989) p. 373.
9. OPAL Collab., P.D. Acton *et al.*, Z. Phys. **C55** (1992) 1.
10. SLD Collab., K. Abe *et al.*, Phys. Rev. **D51** (1995) 962.
11. P.M. Stevenson, Phys. Rev. **D23** (1981) 2916.
12. G. Grunberg, Phys. Rev. **D29** (1984) 2315.
13. S.J. Brodsky, G.P. Lepage, P.B. Mackenzie, Phys. Rev. **D28** (1983) 228.
14. M.A. Samuel, G. Li, E. Steinfelds, Phys. Rev. **D48** (1993) 869.
15. M.A. Samuel, G. Li, E. Steinfelds, Phys. Rev. **E51** (1995) 3911.
16. See *eg.* G.A. Baker Jr., ‘Essentials of Padé Approximants’, Academic Press, 1975.

17. M.A. Samuel, J. Ellis, M. Karliner, Phys. Rev. Lett. **73** (1994) 1207.

18. J. Ellis *et al.*, Phys. Lett. **B366** (1996) 268.

19. H. Masuda, Y. Ohnishi, SLAC-PUB-6560 (1994); subm. to Phys. Rev. D.

20. EVENT program supplied by P. Nason.

21. See *eg.*, Yu.L. Dokshitzer, G. Marchesini, B.R. Webber, CERN-TH/95-281 (1995).

22. P.N. Burrows, SLAC-PUB-7093 (1996); To appear in Proc. Workshop on Physics and Experiments with Linear Colliders, September 8-12 1995, Morioka-Appi, Iwate, Japan.

Observable	value X	$A(X)$	$B(X)$	$B(X)/A(X)$	$C(X)$
τ	0.18	23.93	711.1	29.7	21130
ρ	0.15	36.55	624.5	17.1	10670
B_T	0.23	21.69	1042	48.0	50020
B_W	0.14	82.16	1402	17.1	23940
O	0.21	71.27	-363.0	-5.09	1848
C	0.46	18.89	518.9	27.8	14260
y_c (D_2^E)	0.17	38.84	1217	31.3	38140
y_c (D_2^{E0})	0.17	38.84	822.1	21.2	17400
y_c (D_2^P)	0.12	78.10	1029	13.2	13550
y_c (D_2^{P0})	0.17	38.84	601.6	15.5	9318
y_c (D_2^D)	0.12	33.10	490.6	14.8	7271
y_c (D_2^G)	0.22	37.93	412.7	10.9	4489
χ (EEC)	91.8°	2.460	44.23	18.0	795
χ $(AEEC)$	41.4°	2.682	22.74	8.48	193
χ $(JCEF)$	131.4°	5.196	50.97	9.81	500

Table 1. Perturbative QCD calculation of $1/\sigma d\sigma/dX$ for each observable (first column) at a representative value X (second column). The third and fourth columns show the leading and next-to-leading order coefficients, respectively. The ratio of coefficients is shown in the fifth column, and the PA [0/1] prediction for the next-to-next-to-leading order coefficient $C(X)$ is listed in the sixth column.

Observable	$\alpha_s(M_Z^2)$	χ^2_{dof}
τ	0.1172±0.0009	0.6
ρ	0.1183±0.0007	0.9
B_T	0.1031±0.0009	112
B_W	0.1143±0.0008	1.6
O	0.1230±0.0011	0.6
C	0.1158±0.0008	2.7
D_2^E	0.1164±0.0006	6.4
D_2^{E0}	0.1105±0.0007	3.5
D_2^P	0.1144±0.0008	0.8
D_2^{P0}	0.1122±0.0009	3.4
D_2^D	0.1156±0.0011	4.0
D_2^G	0.1122±0.0008	3.9
EEC	0.1154±0.0008	0.4
$AEEC$	0.1082±0.0012	0.4
$JCEF$	0.1124±0.0007	0.2

Table 2. Values of $\alpha_s(M_Z^2)$ and χ^2_{dof} from fits of QCD predictions incorporating the PA [0/1] estimate for the O(α_s^3) term. The errors are statistical only and are highly correlated between observables.

Figure Caption

FIG. 1. Values of $\alpha_s(M_Z^2)$ determined from fits to event shape observables (see text): (a) $\mathrm{O}(\alpha_s^2)$ (circles); (b) $\mathrm{O}(\alpha_s^3)$ estimate (squares); (c) Padé sum (PS) (crosses). The shaded band shown for each observable is dominated by the renormalisation scale uncertainty on the $\mathrm{O}(\alpha_s^2)$ fit. For each point combined experimental statistical and systematic errors [10] are shown; the errors are highly correlated between observables.