4 CoLoRFulNNLO at work: a determination of $\alpha_{\rm S}$

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4.1 Introduction

The most precise determination of fundamental parameters of the Standard Model is very important. One such fundamental parameter is the strong coupling of QCD. Its importance can be gauged by taking a look at the various experiments and configurations where it was measured; for an up-to-date summary, see Ref. [1]. The precise measurement of such a parameter is difficult for two reasons. First, high-quality data with small and well-controlled uncertainties are needed. Second, high-precision calculations are needed from the theory side, such that theoretical uncertainties are small as well.

In a theoretical prediction based on calculation in perturbation theory, the uncertainty has two main sources: the omission of higher-order terms, which are estimated by the renormalization scale, and the numerical stability of the integrations. While the dependence on unphysical scales can, in principle, be decreased by including more and more higher-order contributions in the prediction, the numerical uncertainty can be intrinsic to the method used to obtain the theoretical prediction. Moreover, the method of comparing experiment with theory is also affected by another uncertainty. While an experiment measures colour singlet objects, hadrons, the predictions are made in QCD for colourful ones, partons. The assumption of local partonhadron duality ensures a correspondence between these two up to non-perturbative effects. Non-perturbative effects are power corrections in nature, going with some negative power of the collision energy. This means that, for an accurate comparison, either (i) these effects should be estimated and taken into account, or (ii) the experiment should have a high enough energy that these contributions become negligible compared with other effects, or (iii) an observable must be chosen that is not sensitive to these effects.

To take these non-perturbative effects into account, we must choose from phenomenological [2,3] or analytical models [4]. It is worth noting that none of these models is derived from first principles; hence, there is still room for improvement. Non-perturbative effects derived from first principles would also be favoured because these corrections are to be used in comparisons of predictions with experimental measurements. Currently, phenomenological models use several parameters fitted to experimental data; thus, bias is introduced in the measurement of physical parameters. The calculation of non-perturbative corrections from first principles is also advocated because the only available analytical model seems to be ill-suited for the current precision of theoretical calculations, as shown in Ref. [5].

In this report, we show two approaches to how the measurement of a physical parameter, the strong coupling, can be carried out with high precision. Because the used observables allow for such measurements, these can be considered as interesting subjects to study in a future

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Fig. B.4.1: Top: Fixed-order prediction for EEC in the first three orders of perturbation theory with theoretical uncertainties. The dots show the measurement by the OPAL collaboration [11]. Bottom: Comparison of the predictions and the measurement with the NNLO result.

electron-positron collider.

4.2 Precision through higher orders

A possible approach to increasing the precision of a measurement from the theoretical perspective is to select an observable and refine its prediction by including higher-order contributions in fixed-order perturbation theory or by means of resummation. With the completion of the CoLoRFulNNLO subtraction method [6–8] for electron–positron collisions, the next-to-next-toleading-order (NNLO) QCD prediction for energy–energy correlation (EEC) recently became available [9] for the first time. Matching this with predictions obtained by resumming leading (LL), next-to-leading (NLL), and next-to-next-to-leading logarithms (NNLL) in the back-toback region [10], it was possible, by matching the two calculations, to arrive at the most precise theoretical prediction for this observable at NNLO+NNLL accuracy in QCD [5]. The energy– energy correlation is defined as a normalised energy-weighted sum of two-particle correlations:

$$\frac{1}{\sigma_{\rm t}} \frac{\mathrm{d}\Sigma(\chi)}{\mathrm{d}\cos\chi} \equiv \frac{1}{\sigma_{\rm t}} \int \sum_{i,j} \frac{E_i E_j}{Q^2} \mathrm{d}\sigma_{\mathrm{e^+e^-} \to ij+X} \delta(\cos\chi + \cos\theta_{ij}), \qquad (4.1)$$

where Q is the centre-of mass energy of the collision, σ_t is the corresponding total cross-section, E_i is the energy of the *i*th particle, and $\cos \theta_{ij}$ is the enclosed angle between particles *i* and *j*. The theoretical prediction for EEC in the first three orders of perturbation theory is depicted in Fig. B.4.1. The theoretical uncertainties were obtained by varying the renormalization scale between $m_Z/2$ and $2m_Z$. As can be seen from the lower panel, even when using the highestprecision prediction, the difference between measurement and theory is sizeable. This can be attributed to missing higher-order terms becoming important at the edge of phase space and missing hadronization corrections.

The behaviour near $\chi = 0$ can be improved by including all-order results through resummation. As described in Ref. [12], we used modern Monte Carlo (MC) tools to extract such



Fig. B.4.2: EEC distributions obtained with the two MC tools at the parton and hadron level at 91.2 GeV, with corresponding OPAL data. Note that for these two plots a different definition of χ was used: this time, the back-to-back region corresponds to $\chi \to 180^{\circ}$.

corrections for EEC. To do this, we generated event samples at both the hadron and the parton level and the ratio of these provided the hadron-to-parton ratio or H/P. Using this ratio and multiplying our parton-level predictions bin by bin, we obtained our theoretical prediction at the hadron level. As MC tools, we used SHERPA2.2.4 [13] and Herwig7.1.1 [14]. The exact set-up of the MC tools is presented in Ref. [12].

The value for the strong coupling was determined by fitting the predictions to 20 different datasets (for details, see Table 1 of Ref. [12]). For illustrative purposes, Fig. B.4.2 shows the predictions obtained with SHERPA and Herwig at the parton and hadron level. For SHERPA, we used both the Lund (S^{L}) [3] and cluster (S^{C}) [2] hadronization models, while in Herwig we used the built-in cluster model. The figure also indicates the range used in the actual fitting procedure.

For the fitting, the MINUIT2 program [15] was used to minimize the quantity:

$$\chi^2(\alpha_{\rm S}) = \sum_{\rm datasets} \chi^2_{\rm dataset}(\alpha_{\rm S}) \tag{4.2}$$

with the $\chi^2(\alpha_{\rm S})^{\dagger}$ quantity calculated as:

$$\chi^{2}(\alpha_{\rm S}) = (\boldsymbol{D} - \boldsymbol{P}(\alpha_{\rm S}))^{\rm T} \underline{\underline{V}}^{-1} (\boldsymbol{D} - \boldsymbol{P}(\alpha_{\rm S})), \qquad (4.3)$$

where D is the vector of data points, P is the vector of predictions as functions of $\alpha_{\rm S}$ and $\underline{\underline{V}}$ is the covariance matrix.

[†]Not to be confused with the angle χ .

With the fitting procedure performed in the range between 60° and 160°. The resulting strong coupling NNLL+NNLO prediction is

$$\alpha_{\rm S}(m_{\rm Z}) = 0.117\,50 \pm 0.002\,87\tag{4.4}$$

and at NNLL+NLO accuracy is

$$\alpha_{\rm S}(m_{\rm Z}) = 0.122\,00 \pm 0.005\,35\,. \tag{4.5}$$

Notice the reduction in uncertainty as we go from NNLL+NLO to NNLL+NNLO.

4.3 Precision through small power corrections

As outlined in the introduction, the current methods of taking the effect of non-perturbative contributions into account can raise concerns, mainly because only phenomenological models are present for them. The other big concern is that these models rely on experimental results through tuned parameters. The best option, without any model derived from first principles, is to decrease these effects as much as possible. The idea is simple: if the non-perturbative contribution can be shrunk, its large uncertainties will make a smaller contribution to the final uncertainty of the extracted value of the strong coupling.

In this section, we focus on altering the definitions of existing observables to decrease the non-perturbative corrections. The most basic and most used observables in electron-positron collisions are the thrust (T) and the various jet masses. In their original definitions, these all incorporate all registered hadronic objects of the event or a given, well-defined region. Hence, a natural way to modify them is to filter the tracks contributing to their value in an event. One possible way to remove tracks is by means of grooming [16–21]. In particular, the soft drop [21] is a grooming when a part of the soft content of the event is removed according to some criteria.

In Ref. [22], soft-drop variants were defined for thrust, $\tau'_{SD} = 1 - T'_{SD}$, hemisphere jet mass, $e_2^{(2)}$ and narrow jet mass, ρ . As showed in that paper, the non-perturbative corrections can be drastically decreased if soft drop is applied. The effect of soft drop turns out to be the most significant in the peak region of the distributions, where the contribution from all-order resummation and non-perturbative effects is the greatest. This makes these observables promising candidates for strong coupling measurements at a future electron–positron collider. The application of these observables—although very interesting—is limited at LEP measurements, owing to the limited amount of data taken and because the soft-drop procedure inherently results in a decrease of cross-section.

In our recent paper [23], we analysed the proposed observables from the standpoint of perturbative behaviour by calculating the NNLO QCD corrections to the observables and analysing their dependence on the non-physical renormalization scale as an indicator of the size of neglected higher-order terms. The soft-drop versions of the observables listed have two parameters related to soft drop: z_c and β [22]. This allows for optimisation in order to minimize the decrease in cross-section when the soft-drop procedure is applied.

Figure B.4.3 shows the soft-dropped thrust distribution in the first three orders of QCD perturbation theory for a specific choice of the two soft-drop related parameters. On the right-hand side of the figure, the K factors are depicted for various parameter choices to illustrate the stability of the result. We found that the most stable perturbation prediction and moderate drop in cross-section can be achieved when $(z_c, \beta) = (0.1, 0)$.



Fig. B.4.3: Left: Soft-dropped thrust distribution at the Z peak in the first three orders of perturbation theory; the bands represent the uncertainty coming from the variation of the renormalization scale between Q/2 and 2Q. Right: The K factors for the soft-dropped thrust distribution for various choices of the soft-drop parameters.



Fig. B.4.4: The same as Fig. B.4.3 but for the hemisphere jet mass

Figure B.4.4 depicts the soft-dropped hemisphere jet mass in exactly the same way as the soft-dropped thrust shown in Fig. B.4.3. In this case, it can be seen once more that the perturbative behaviour stabilizes on going to higher orders in perturbation theory. This is most pronounced at the left-hand side of the peak, where the NLO and NNLO predictions coincide. For this observable, we found that the best choice for the soft-drop parameters is also $(z_c, \beta) = (0.1, 0)$. For the traditional versions of these observables, the peak region is the one where the all-order resummed results and non-perturbative corrections must have agreement with the experiment, but for the soft-dropped versions neither the higher-order contributions nor the non-perturbative corrections are drastic. The minimal role of higher orders in perturbation theory can be seen from the perturbative stability of our results, while the small size of nonperturbative corrections has been shown in Ref. [22]. These properties make the soft-dropped event shapes attractive observables for the extraction of the strong coupling.

4.4 Conclusions

A future electron-positron collider would be considered a dream machine for many reasons. A machine of this type would allow for a precise tuning of collision energy; it would have no annoying underlying event and it would have coloured partons in the initial state. Several possible measurements could be envisioned at such a machine but from the QCD point of view, determination of the strong coupling stands out. The strong coupling is a fundamental parameter of the Standard Model of particle physics, so knowing its value is of key importance.

In this report, we showed two possible ways to conduct such a measurement. First, it can be achieved by including higher-order corrections in the theoretical prediction and comparing this with the experimental result modelling non-perturbative effects with modern MC tools. Second, we showed modified versions of well-known observables defined in electron–positron collisions where non-perturbative corrections can be minimized, hence diminishing the effects of their uncertainties on theoretical predictions. These observables seem to be promising candidates, not just for strong coupling measurements but also for the purpose of testing the Standard Model further. Thus, they should be seriously considered as important measurements at a future electron–positron facility.

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