

## 9. QUANTUM CHROMODYNAMICS

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### 9.1. Basics

Quantum Chromodynamics (QCD), the gauge field theory that describes the strong interactions of colored quarks and gluons, is the SU(3) component of the SU(3)×SU(2)×U(1) Standard Model of Particle Physics.

The Lagrangian of QCD is given by

$$\mathcal{L} = \sum_q \bar{\psi}_{q,a} (i\gamma^\mu \partial_\mu \delta_{ab} - g_s \gamma^\mu t_{ab}^C \mathcal{A}_\mu^C - m_q \delta_{ab}) \psi_{q,b} - \frac{1}{4} F_{\mu\nu}^A F^{A\mu\nu}, \quad (9.1)$$

where repeated indices are summed over. The  $\gamma^\mu$  are the Dirac  $\gamma$ -matrices. The  $\psi_{q,a}$  are quark-field spinors for a quark of flavor  $q$  and mass  $m_q$ , with a color-index  $a$  that runs from  $a = 1$  to  $N_c = 3$ , *i.e.* quarks come in three “colors.” Quarks are said to be in the fundamental representation of the SU(3) color group.

The  $\mathcal{A}_\mu^C$  correspond to the gluon fields, with  $C$  running from 1 to  $N_c^2 - 1 = 8$ , *i.e.* there are eight kinds of gluon. Gluons are said to be in the adjoint representation of the SU(3) color group. The  $t_{ab}^C$  correspond to eight  $3 \times 3$  matrices and are the generators of the SU(3) group (cf. the section on “SU(3) isoscalar factors and representation matrices” in this *Review* with  $t_{ab}^C \equiv \lambda_{ab}^C/2$ ). They encode the fact that a gluon’s interaction with a quark rotates the quark’s color in SU(3) space. The quantity  $g_s$  is the QCD coupling constant. Finally, the field tensor  $F_{\mu\nu}^A$  is given by

$$F_{\mu\nu}^A = \partial_\mu \mathcal{A}_\nu^A - \partial_\nu \mathcal{A}_\mu^A - g_s f_{ABC} \mathcal{A}_\mu^B \mathcal{A}_\nu^C \quad [t^A, t^B] = i f_{ABC} t^C, \quad (9.2)$$

where the  $f_{ABC}$  are the structure constants of the SU(3) group.

Neither quarks nor gluons are observed as free particles. Hadrons are color-singlet (*i.e.* color-neutral) combinations of quarks, anti-quarks, and gluons.

Ab-initio predictive methods for QCD include lattice gauge theory and perturbative expansions in the coupling. The Feynman rules of QCD involve a quark-antiquark-gluon ( $q\bar{q}g$ ) vertex, a 3-gluon vertex (both proportional to  $g_s$ ), and a 4-gluon vertex (proportional to  $g_s^2$ ). A full set of Feynman rules is to be found for example in Ref. 3.

Useful color-algebra relations include:  $t_{ab}^A t_{bc}^A = C_F \delta_{ac}$ , where  $C_F \equiv (N_c^2 - 1)/(2N_c) = 4/3$  is the color-factor (“Casimir”) associated with gluon emission from a quark;  $f^{ACD} f^{BCD} = C_A \delta_{AB}$  where  $C_A \equiv N_c = 3$  is the color-factor associated with gluon emission from a gluon;  $t_{ab}^A t_{ab}^B = T_R \delta_{AB}$ , where  $T_R = 1/2$  is the color-factor for a gluon to split to a  $q\bar{q}$  pair.

The fundamental parameters of QCD are the coupling  $g_s$  (or  $\alpha_s = \frac{g_s^2}{4\pi}$ ) and the quark masses  $m_q$ .

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There is freedom for an additional CP-violating term to be present in the QCD Lagrangian,  $\theta \frac{\alpha_s}{8\pi} F_{\mu\nu}^A \tilde{F}^{A\mu\nu}$ , where  $F_{\mu\nu}^A \tilde{F}^{A\mu\nu}$  is the dual of the gluon field tensor,  $\frac{1}{2} \epsilon_{\mu\nu\sigma\rho} F^{A\sigma\rho}$ . Experimental limits on the neutron electric dipole moment [1] constrain the coefficient of this contribution to satisfy  $|\theta| \lesssim 10^{-10}$ . Further discussion is to be found in Ref. 2 and Axions section in the Listings of this *Review*.

This section will concentrate mainly on perturbative aspects of QCD as they relate to collider physics. Related textbooks and reviews include Refs. 3–6. Aspects specific to Monte Carlo event generators are reviewed in a dedicated section Chap. 38. Lattice QCD is also reviewed in a section of its own Chap. 17, with additional discussion of non-perturbative aspects to be found in the sections on “Quark Masses”, “The CKM quark-mixing matrix”, “Structure Functions” and event generators in this *Review*. For an overview of some of the QCD issues and recent results in heavy-ion physics, see for example Refs. 7, 8.

### 9.1.1. Running coupling :

In the framework of perturbative QCD (pQCD), predictions for observables are expressed in terms of the renormalized coupling  $\alpha_s(\mu_R^2)$ , a function of an (unphysical) renormalization scale  $\mu_R$ . When one takes  $\mu_R$  close to the scale of the momentum transfer  $Q$  in a given process, then  $\alpha_s(\mu_R^2 \simeq Q^2)$  is indicative of the effective strength of the strong interaction in that process.

The coupling satisfies the following renormalization group equation (RGE):

$$\mu_R^2 \frac{d\alpha_s}{d\mu_R^2} = \beta(\alpha_s) = -(b_0\alpha_s^2 + b_1\alpha_s^3 + b_2\alpha_s^4 + \dots) \quad (9.3)$$

where  $b_0 = (11C_A - 4n_f T_R)/(12\pi) = (33 - 2n_f)/(12\pi)$  is referred to as the 1-loop beta-function coefficient, the 2-loop coefficient is  $b_1 = (17C_A^2 - n_f T_R(10C_A + 6C_F))/(24\pi^2) = (153 - 19n_f)/(24\pi^2)$ , and the 3-loop coefficient is  $b_2 = (2857 - \frac{5033}{9}n_f + \frac{325}{27}n_f^2)/(128\pi^3)$ . The 4-loop coefficient,  $b_3$ , is to be found in Refs. 9, 10<sup>†</sup>. The minus sign in Eq. (9.3) is the origin of Asymptotic Freedom, *i.e.* the fact that the strong coupling becomes weak for processes involving large momentum transfers (“hard processes”),  $\alpha_s \sim 0.1$  for momentum transfers in the 100 GeV – TeV range.

The  $\beta$ -function coefficients, the  $b_i$ , are given for the coupling of an *effective theory* in which  $n_f$  of the quark flavors are considered light ( $m_q \ll \mu_R$ ), and in which the remaining heavier quark flavors decouple from the theory. One may relate the coupling for the theory with  $n_f + 1$  light flavors to that with  $n_f$  flavors through an equation of the form

$$\alpha_s^{(n_f+1)}(\mu_R^2) = \alpha_s^{(n_f)}(\mu_R^2) \left( 1 + \sum_{n=1}^{\infty} \sum_{\ell=0}^n c_{n\ell} [\alpha_s^{(n_f)}(\mu_R^2)]^n \ln^\ell \frac{\mu_R^2}{m_h^2} \right), \quad (9.4)$$

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<sup>†</sup> One should be aware that the  $b_2$  and  $b_3$  coefficients are renormalization-scheme-dependent, and given here in the  $\overline{\text{MS}}$  scheme, as discussed below.

where  $m_h$  is the mass of the  $(n_f+1)^{\text{th}}$  flavor, and the first few  $c_{nl}$  coefficients are  $c_{11} = \frac{1}{6\pi}$ ,  $c_{10} = 0$ ,  $c_{22} = c_{11}^2$ ,  $c_{21} = \frac{19}{24\pi^2}$ , and  $c_{20} = -\frac{11}{72\pi^2}$  when  $m_h$  is the  $\overline{\text{MS}}$  mass at scale  $m_h$  ( $c_{20} = \frac{7}{24\pi^2}$  when  $m_h$  is the pole mass — mass definitions are discussed below and in the review on “Quark Masses”). Terms up to  $c_{4\ell}$  are to be found in Refs. 11, 12. Numerically, when one chooses  $\mu_R = m_h$ , the matching is a modest effect, owing to the zero value for the  $c_{10}$  coefficient. Relations between  $n_f$  and  $(n_f+2)$  flavors where the two heavy flavors are close in mass are given to three loops in Ref. 13.

Working in an energy range where the number of flavors is taken constant, a simple exact analytic solution exists for Eq. (9.3) only if one neglects all but the  $b_0$  term, giving  $\alpha_s(\mu_R^2) = (b_0 \ln(\mu_R^2/\Lambda^2))^{-1}$ . Here  $\Lambda$  is a constant of integration, which corresponds to the scale where the perturbatively-defined coupling would diverge, *i.e.* it is the non-perturbative scale of QCD. A convenient approximate analytic solution to the RGE that includes also the  $b_1$ ,  $b_2$ , and  $b_3$  terms is given by (see for example Ref. 14),

$$\alpha_s(\mu_R^2) \simeq \frac{1}{b_0 t} \left( 1 - \frac{b_1}{b_0^2} \frac{\ln t}{t} + \frac{b_1^2(\ln^2 t - \ln t - 1) + b_0 b_2}{b_0^4 t^2} - \frac{b_1^3(\ln^3 t - \frac{5}{2} \ln^2 t - 2 \ln t + \frac{1}{2}) + 3b_0 b_1 b_2 \ln t - \frac{1}{2} b_0^2 b_3}{b_0^6 t^3} \right), \quad t \equiv \ln \frac{\mu_R^2}{\Lambda^2}, \quad (9.5)$$

again parametrized in terms of a constant  $\Lambda$ . Note that Eq. (9.5) is one of several possible approximate 4-loop solutions for  $\alpha_s(\mu_R^2)$ , and that a value for  $\Lambda$  only defines  $\alpha_s(\mu_R^2)$  once one knows which particular approximation is being used. An alternative to the use of formulas such as Eq. (9.5) is to solve the RGE exactly, numerically (including the discontinuities, Eq. (9.4), at flavor thresholds). In such cases the quantity  $\Lambda$  is not defined at all. For these reasons, in determinations of the coupling, it has become standard practice to quote the value of  $\alpha_s$  at a given scale (typically  $M_Z$ ) rather than to quote a value for  $\Lambda$ .

The value of the coupling, as well as the exact forms of the  $b_2$ ,  $c_{10}$  (and higher order) coefficients, depend on the renormalization scheme in which the coupling is defined, *i.e.* the convention used to subtract infinities in the context of renormalization. The coefficients given above hold for a coupling defined in the modified minimal subtraction ( $\overline{\text{MS}}$ ) scheme [15], by far the most widely used scheme.

A discussion of determinations of the coupling and a graph illustrating its scale dependence (“running”) are to be found in Section 9.3.4.

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### 9.1.2. Quark masses :

Free quarks are never observed, *i.e.* a quark never exists on its own for a time longer than  $\sim 1/\Lambda$ : up, down, strange, charm, and bottom quarks all *hadronize*, *i.e.* become part of a meson or baryon, on a timescale  $\sim 1/\Lambda$ ; the top quark instead decays before it has time to hadronize. This means that the question of what one means by the quark mass is a complex one, which requires that one adopts a specific prescription. A perturbatively defined prescription is the pole mass,  $m_q$ , which corresponds to the position of the divergence of the propagator. This is close to one's physical picture of mass. However, when relating it to observable quantities, it suffers from substantial non-perturbative ambiguities (see *e.g.* Ref. 16). An alternative is the  $\overline{\text{MS}}$  mass,  $\overline{m}_q(\mu_R^2)$ , which depends on the renormalization scale  $\mu_R$ .

Results for the masses of heavier quarks are often quoted either as the pole mass or as the  $\overline{\text{MS}}$  mass evaluated at a scale equal to the mass,  $\overline{m}_q(\overline{m}_q^2)$ ; light quark masses are generally quoted in the  $\overline{\text{MS}}$  scheme at a scale  $\mu_R \sim 2 \text{ GeV}$ . The pole and  $\overline{\text{MS}}$  masses are related by a slowly converging series that starts  $m_q = \overline{m}_q(\overline{m}_q^2)(1 + \frac{4\alpha_s(\overline{m}_q^2)}{3\pi} + \mathcal{O}(\alpha_s^2))$ , while the scale-dependence of  $\overline{\text{MS}}$  masses is given by

$$\mu_R^2 \frac{d\overline{m}_q(\mu_R^2)}{d\mu_R^2} = \left[ -\frac{\alpha_s(\mu_R^2)}{\pi} + \mathcal{O}(\alpha_s^2) \right] \overline{m}_q(\mu_R^2). \quad (9.6)$$

More detailed discussion is to be found in a dedicated section of the *Review*, “Quark Masses.”

## 9.2. Structure of QCD predictions

### 9.2.1. Fully inclusive cross sections :

The simplest observables in QCD are those that do not involve initial-state hadrons and that are fully inclusive with respect to details of the final state. One example is the total cross section for  $e^+e^- \rightarrow \text{hadrons}$  at center-of-mass energy  $Q$ , for which one can write

$$\frac{\sigma(e^+e^- \rightarrow \text{hadrons}, Q)}{\sigma(e^+e^- \rightarrow \mu^+\mu^-, Q)} \equiv R(Q) = R_{\text{EW}}(Q)(1 + \delta_{\text{QCD}}(Q)), \quad (9.7)$$

where  $R_{\text{EW}}(Q)$  is the purely electroweak prediction for the ratio and  $\delta_{\text{QCD}}(Q)$  is the correction due to QCD effects. To keep the discussion simple, we can restrict our attention to energies  $Q \ll M_Z$ , where the process is dominated by photon exchange ( $R_{\text{EW}} = 3 \sum_q e_q^2$ , neglecting finite-quark-mass corrections),

$$\delta_{\text{QCD}}(Q) = \sum_{n=1}^{\infty} c_n \cdot \left( \frac{\alpha_s(Q^2)}{\pi} \right)^n + \mathcal{O}\left(\frac{\Lambda^4}{Q^4}\right). \quad (9.8)$$

The first four terms in the  $\alpha_s$  series expansion are then to be found in Refs. 17, 18

$$c_1 = 1, \quad c_2 = 1.9857 - 0.1152n_f, \quad (9.9a)$$

$$c_3 = -6.63694 - 1.20013n_f - 0.00518n_f^2 - 1.240\eta \quad (9.9b)$$

$$c_4 = -156.61 + 18.77n_f - 0.7974n_f^2 + 0.0215n_f^3 + C\eta, \quad (9.9c)$$

with  $\eta = (\sum e_q)^2 / (3 \sum e_q^2)$  and where the coefficient  $C$  of the  $\eta$ -dependent piece in the  $\alpha_s^4$  term has yet to be determined. For corresponding expressions including also  $Z$  exchange and finite-quark-mass effects, see Refs. 19, 20.

A related series holds also for the QCD corrections to the hadronic decay width of the  $\tau$  lepton, which essentially involves an integral of  $R(Q)$  over the allowed range of invariant masses of the hadronic part of the  $\tau$  decay (see e.g. Ref. 17). The series expansions for QCD corrections to Higgs-boson (partial) decay widths are summarized in Refs. 21, 22.

One characteristic feature of Eqs. (9.8) and (9.9) is that the coefficients of  $\alpha_s^n$  increase rapidly order by order: calculations in perturbative QCD tend to converge more slowly than would be expected based just on the size of  $\alpha_s^{\dagger\dagger}$ . Another feature is the existence of an extra ‘‘power-correction’’ term  $\mathcal{O}(\Lambda^4/Q^4)$  in Eq. (9.8), which accounts for contributions that are fundamentally non-perturbative. All high-energy QCD predictions involve such corrections, though the exact power of  $\Lambda/Q$  depends on the observable.

**Scale dependence.** In Eq. (9.8) the renormalization scale for  $\alpha_s$  has been chosen equal to  $Q$ . The result can also be expressed in terms of the coupling at an arbitrary renormalization scale  $\mu_R$ ,

$$\delta_{\text{QCD}}(Q) = \sum_{n=1}^{\infty} \bar{c}_n \left( \frac{\mu_R^2}{Q^2} \right) \cdot \left( \frac{\alpha_s(\mu_R^2)}{\pi} \right)^n + \mathcal{O} \left( \frac{\Lambda^4}{Q^4} \right), \quad (9.10)$$

where  $\bar{c}_1(\mu_R^2/Q^2) \equiv c_1$ ,  $\bar{c}_2(\mu_R^2/Q^2) = c_2 + \pi b_0 c_1 \ln(\mu_R^2/Q^2)$ ,  $\bar{c}_3(\mu_R^2/Q^2) = c_3 + (2b_0 c_2 \pi + b_1 c_1 \pi^2) \ln(\mu_R^2/Q^2) + b_0^2 c_1 \pi^2 \ln^2(\mu_R^2/Q^2)$ , *etc.*. Given an infinite number of terms in the  $\alpha_s$  expansion, the  $\mu_R$  dependence of the  $\bar{c}_n(\mu_R^2/Q^2)$  coefficients will exactly cancel that of  $\alpha_s(\mu_R^2)$ , and the final result will be independent of the choice of  $\mu_R$ : physical observables do not depend on unphysical scales.

With just terms up to  $n = N$ , a residual  $\mu_R$  dependence will remain, which implies an uncertainty on the prediction of  $R(Q)$  due to the arbitrariness of the scale choice. This uncertainty will be  $\mathcal{O}(\alpha_s^{N+1})$ , *i.e.* of the same order as the neglected terms. For this reason it is standard to use QCD predictions’ scale dependence as an estimate of the uncertainties due to neglected terms. One usually takes a central value for  $\mu_R \sim Q$ , in order to avoid the poor convergence of the perturbative series that results from the large  $\ln^{n-1}(\mu_R^2/Q^2)$  terms in the  $\bar{c}_n$  coefficients when  $\mu_R \ll Q$  or  $\mu_R \gg Q$ .

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<sup>††</sup> The situation is significantly worse near thresholds, e.g. the  $t\bar{t}$  production threshold. An overview of some of the effective field theory techniques used in such cases is to be found for example in Ref. 23.

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### 9.2.1.1. Processes with initial-state hadrons:

**Deep Inelastic Scattering.** To illustrate the key features of QCD cross sections in processes with initial-state hadrons, let us consider deep-inelastic scattering (DIS),  $ep \rightarrow e + X$ , where an electron  $e$  with four-momentum  $k$  emits a highly off-shell photon (momentum  $q$ ) that interacts with the proton (momentum  $p$ ). For photon virtualities  $Q^2 \equiv -q^2$  far above the squared proton mass (but far below the  $Z$  mass), the differential cross section in terms of the kinematic variables  $Q^2$ ,  $x = Q^2/(2p \cdot q)$  and  $y = (q \cdot p)/(k \cdot p)$  is

$$\frac{d^2\sigma}{dx dQ^2} = \frac{4\pi\alpha}{2xQ^4} \left[ (1 + (1-y)^2)F_2(x, Q^2) - y^2 F_L(x, Q^2) \right], \quad (9.11)$$

where  $\alpha$  is the electromagnetic coupling and  $F_2(x, Q^2)$  and  $F_L(x, Q^2)$  are proton structure functions, which encode the interaction between the photon (in given polarization states) and the proton. In the presence of parity-violating interactions (e.g.  $\nu p$  scattering) an additional  $F_3$  structure function is present. For an extended review, including equations for the full electroweak and polarized cases, see Sec. 18 of this *Review*.

Structure functions are not calculable in perturbative QCD, nor is any other cross section that involves initial-state hadrons. To zeroth order in  $\alpha_s$ , the structure functions are given directly in terms of non-perturbative parton (quark or gluon) distribution functions (PDFs),

$$F_2(x, Q^2) = x \sum_q e_q^2 f_{q/p}(x), \quad F_L(x, Q^2) = 0, \quad (9.12)$$

where  $f_{q/p}(x)$  is the PDF for quarks of type  $q$  inside the proton, *i.e.* the number density of quarks of type  $q$  inside a fast-moving proton that carry a fraction  $x$  of its longitudinal momentum (the quark flavor index  $q$ , here, is not to be confused with the photon momentum  $q$  in the lines preceding Eq. (9.11)). Since PDFs are non-perturbative, and difficult to calculate in lattice QCD [24], they must be extracted from data.

The above result, with PDFs  $f_{q/p}(x)$  that are independent of the scale  $Q$ , corresponds to the “quark-parton model” picture in which the photon interacts with point-like free quarks, or equivalently, one has incoherent elastic scattering between the electron and individual constituents of the proton. As a consequence, in this picture also  $F_2$  and  $F_L$  are independent of  $Q$ . When including higher orders in pQCD, Eq. (9.12) becomes

$$\begin{aligned} F_2(x, Q^2) = & \\ & x \sum_{n=0}^{\infty} \frac{\alpha_s^n(\mu_R^2)}{(2\pi)^n} \sum_{i=q,g} \int_x^1 \frac{dz}{z} C_{2,i}^{(n)}(z, Q^2, \mu_R^2, \mu_F^2) f_{i/p}\left(\frac{x}{z}, \mu_F^2\right) \\ & + \mathcal{O}\left(\frac{\Lambda^2}{Q^2}\right). \end{aligned} \quad (9.13)$$

Just as in Eq. (9.10), we have a series in powers  $\alpha_s(\mu_R^2)$ , each term involving a coefficient  $C_{2,i}^{(n)}$  that can be calculated using Feynman graphs. An important difference relative to

Eq. (9.10) stems from the fact that the quark's momentum, when it interacts with the photon, can differ from its momentum when it was extracted from the proton, because it may have radiated gluons in between. As a result, the  $C_{2,i}^{(n)}$  coefficients are functions that depend on the ratio,  $z$ , of these two momenta, and one must integrate over  $z$ . At zeroth order,  $C_{2,q}^{(0)} = e_q^2 \delta(1-z)$  and  $C_{2,g}^{(0)} = 0$ .

The majority of the emissions that modify a parton's momentum are collinear (parallel) to that parton, and don't depend on the fact that the parton is destined to interact with a photon. It is natural to view these emissions as modifying the proton's structure rather than being part of the coefficient function for the parton's interaction with the photon. Technically, one uses a procedure known as *collinear factorization* to give a well-defined meaning to this distinction, most commonly through the  $\overline{\text{MS}}$  factorization scheme, defined in the context of dimensional regularization. The  $\overline{\text{MS}}$  factorization scheme involves an arbitrary choice of *factorization scale*,  $\mu_F$ , whose meaning can be understood roughly as follows: emissions with transverse momenta above  $\mu_F$  are included in the  $C_{2,q}^{(n)}(z, Q^2, \mu_R^2, \mu_F^2)$ ; emissions with transverse momenta below  $\mu_F$  are accounted for within the PDFs,  $f_{i/p}(x, \mu_F^2)$ . While collinear factorization is generally believed to be valid for suitable (sufficiently inclusive) observables in processes with hard scales, Ref. 35, which reviews the factorization proofs in detail, is cautious in the statements it makes about their exhaustivity, notably for the hadron-collider processes that we shall discuss below. Further discussion is to be found in Refs. 36,37.

The PDFs' resulting dependence on  $\mu_F$  is described by the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) equations [25], which to leading order (LO) read\*

$$\mu^2 \frac{\partial f_{i/p}(x, \mu_F^2)}{\partial \mu_F^2} = \sum_j \frac{\alpha_s(\mu_F^2)}{2\pi} \int_x^1 \frac{dz}{z} P_{i \leftarrow j}^{(1)}(z) f_{j/p}\left(\frac{x}{z}, \mu_F^2\right), \quad (9.14)$$

with, for example,  $P_{q \leftarrow g}^{(1)}(z) = T_R(z^2 + (1-z)^2)$ . The other LO splitting functions are listed in Sec. 18 of this *Review*, while results up to next-to-leading order (NLO),  $\alpha_s^2$ , and next-to-next-to-leading order (NNLO),  $\alpha_s^3$ , are given in Refs. 26 and 27 respectively. The coefficient functions are also  $\mu_F$  dependent, for example  $C_{2,i}^{(1)}(x, Q^2, \mu_R^2, \mu_F^2) = C_{2,i}^{(1)}(x, Q^2, \mu_R^2, Q^2) - \ln(\frac{\mu_F^2}{Q^2}) \sum_j \int_x^1 \frac{dz}{z} C_{2,j}^{(0)}(\frac{x}{z}) P_{j \leftarrow i}^{(1)}(z)$ . For the electromagnetic component of DIS with light quarks and gluons they are known to  $\mathcal{O}(\alpha_s^3)$  (N<sup>3</sup>LO) [28]. For weak currents they are known fully to  $\alpha_s^2$  (NNLO) [29] with

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\* LO is generally taken to mean the lowest order at which a quantity is non-zero. This definition is nearly always unambiguous, the one major exception being for the case of the hadronic branching ratio of virtual photons,  $Z$ ,  $\tau$ , etc., for which two conventions exist: LO can either mean the lowest order that contributes to the hadronic branching fraction, *i.e.* the term “1” in Eq. (9.7); or it can mean the lowest order at which the hadronic branching ratio becomes sensitive to the coupling,  $n = 1$  in Eq. (9.8), as is relevant when extracting the value of the coupling from a measurement of the branching ratio. Because of this ambiguity, we avoided use of the term “LO” in that context.

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substantial results known also at N<sup>3</sup>LO [30]. For heavy quark production they are known to  $\mathcal{O}(\alpha_s^2)$  [31] (NLO insofar as the series starts at  $\mathcal{O}(\alpha_s)$ ), with work ongoing towards NNLO [32,33].

As with the renormalization scale, the choice of factorization scale is arbitrary, but if one has an infinite number of terms in the perturbative series, the  $\mu_F$ -dependences of the coefficient functions and PDFs will compensate each other fully. Given only  $N$  terms of the series, a residual  $\mathcal{O}(\alpha_s^{N+1})$  uncertainty is associated with the ambiguity in the choice of  $\mu_F$ . As with  $\mu_R$ , varying  $\mu_F$  provides an input in estimating uncertainties on predictions. In inclusive DIS predictions, the default choice for the scales is usually  $\mu_R = \mu_F = Q$ .

**Hadron-hadron collisions.** The extension to processes with two initial-state hadrons is straightforward, and for example the total (inclusive) cross section for  $W$  boson production in collisions of hadrons  $h_1$  and  $h_2$  can be written as

$$\begin{aligned} \sigma(h_1 h_2 \rightarrow W + X) &= \sum_{n=0}^{\infty} \alpha_s^n(\mu_R^2) \sum_{i,j} \int dx_1 dx_2 f_{i/h_1}(x_1, \mu_F^2) f_{j/h_2}(x_2, \mu_F^2) \\ &\times \hat{\sigma}_{ij \rightarrow W+X}^{(n)}(x_1 x_2 s, \mu_R^2, \mu_F^2), \end{aligned} \quad (9.15)$$

where  $s$  is the squared center-of-mass energy of the collision. At LO,  $n = 0$ , the hard (partonic) cross section  $\hat{\sigma}_{ij \rightarrow W+X}^{(0)}(x_1 x_2 s, \mu_R^2, \mu_F^2)$  is simply proportional to  $\delta(x_1 x_2 s - M_W^2)$ , in the narrow  $W$ -boson width approximation (see Sec. 44 of this *Review* for detailed expressions for this and other hard scattering cross sections). It is non-zero only for choices of  $i, j$  that can directly give a  $W$ , such as  $i = u, j = \bar{d}$ . At higher orders,  $n \geq 1$ , new partonic channels contribute, such as  $gq$ , and there is no restriction  $x_1 x_2 s = M_W^2$ .

Equation 9.15 involves a collinear factorization between hard cross section and PDFs, just like Eq. (9.13). As long as the same factorization scheme is used in DIS and  $pp$  or  $p\bar{p}$  (usually the  $\overline{\text{MS}}$  scheme), then PDFs extracted in DIS can be directly used in  $pp$  and  $p\bar{p}$  predictions [34,35] (with the anti-quark distributions in an anti-proton being the same as the quark distributions in a proton). Note that Eq. (9.15) only holds to within contributions that are suppressed by powers of  $m_p^2/m_W^2$ .

Fully inclusive hard cross sections are known to NNLO, i.e. corrections up to relative order  $\alpha_s^2$ , for Drell-Yan (DY) lepton-pair and vector-boson production [38,39], Higgs-boson production via gluon fusion [39–41], Higgs-boson production in association with a vector boson [42] and Higgs-boson production via vector-boson fusion [43] (in an approximation that factorizes the production of the two vector bosons). A review of fully inclusive Higgs-related results is to be found in Ref. 44.

**Photoproduction.**  $\gamma p$  (and  $\gamma\gamma$ ) collisions are similar to  $pp$  collisions, with the subtlety that the photon can behave in two ways: there is “direct” photoproduction, in which the photon behaves as a point-like particle and takes part directly in the hard collision, with hard subprocesses such as  $\gamma g \rightarrow q\bar{q}$ ; there is also resolved photoproduction, in which



the photon behaves like a hadron, with non-perturbative partonic substructure and a corresponding PDF for its quark and gluon content,  $f_{i/\gamma}(x, Q^2)$ .

While useful to understand the general structure of  $\gamma p$  collisions, the distinction between direct and resolved photoproduction is not well defined beyond leading order, as discussed for example in Ref. 45.

**The high-energy limit.** In situations in which the total center-of-mass energy  $\sqrt{s}$  is much larger than other scales in the problem (*e.g.*  $Q$  in DIS,  $m_b$  for  $b\bar{b}$  production in  $pp$  collisions, *etc.*), each power of  $\alpha_s$  beyond LO can be accompanied by a power of  $\ln(s/Q^2)$  (or  $\ln(s/m_b^2)$ , *etc.*). This is known as the high-energy or Balitsky-Fadin-Kuraev-Lipatov (BFKL) limit [46–48]. Currently it is possible to account for the dominant and first subdominant [49,50] power of  $\ln s$  at each order of  $\alpha_s$ , and also to estimate further subdominant contributions that are numerically large (see Refs. 51–53 and references therein).

Physically, the summation of all orders in  $\alpha_s$  can be understood as leading to a growth with  $s$  of the gluon density in the proton. At sufficiently high energies this implies non-linear effects, whose treatment has been the subject of intense study (see for example Refs. 54, 55 and references thereto). Note that it is not straightforward to relate these results to the genuinely non-perturbative total, elastic and diffractive cross sections for hadron-hadron scattering (experimental results for which are summarized in section Chap. 46 of this *Review*).

### 9.2.2. *Non fully inclusive cross-sections :*

QCD final states always consist of hadrons, while perturbative QCD calculations deal with partons. Physically, an energetic parton fragments (“showers”) into many further partons, which then, on later timescales, undergo a transition to hadrons (“hadronization”). Fixed-order perturbation theory captures only a small part of these dynamics.

This does not matter for the fully inclusive cross sections discussed above: the showering and hadronization stages are “unitary”, *i.e.* they do not change the overall probability of hard scattering, because they occur long after it has taken place.

Less inclusive measurements, in contrast, may be affected by the extra dynamics. For those sensitive just to the main directions of energy flow (jet rates, event shapes, cf. Sec. 9.3.1) fixed order perturbation theory is often still adequate, because showering and hadronization don’t substantially change the overall energy flow. This means that one can make a prediction using just a small number of partons, which should correspond well to a measurement of the same observable carried out on hadrons. For observables that instead depend on distributions of individual hadrons (which, *e.g.*, are the inputs to detector simulations), it is mandatory to account for showering and hadronization. The range of predictive techniques available for QCD final states reflects this diversity of needs of different measurements.

While illustrating the different methods, we shall for simplicity mainly use expressions that hold for  $e^+e^-$  scattering. The extension to cases with initial-state partons will be mostly straightforward (space constraints unfortunately prevent us from addressing

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diffraction and exclusive hadron-production processes; extensive discussion is to be found in Refs. 56, 57).

### 9.2.2.1. Preliminaries: Soft and collinear limits:

Before examining specific predictive methods, it is useful to be aware of a general property of QCD matrix elements in the soft and collinear limits. Consider a squared tree-level matrix element  $|M_n^2(p_1, \dots, p_n)|$  for the process  $e^+e^- \rightarrow n$  partons with momenta  $p_1, \dots, p_n$ , and a corresponding phase-space integration measure  $d\Phi_n$ . If particle  $n$  is a gluon, and additionally it becomes collinear (parallel) to another particle  $i$  and its momentum tends to zero (it becomes “soft”), the matrix element simplifies as follows,

$$\begin{aligned} \lim_{\theta_{in} \rightarrow 0, E_n \rightarrow 0} d\Phi_n |M_n^2(p_1, \dots, p_n)| \\ = d\Phi_{n-1} |M_{n-1}^2(p_1, \dots, p_{n-1})| \frac{\alpha_s C_i}{\pi} \frac{d\theta_{in}^2}{\theta_{in}^2} \frac{dE_n}{E_n}, \end{aligned} \quad (9.16)$$

where  $C_i = C_F$  ( $C_A$ ) if  $i$  is a quark (gluon). This formula has non-integrable divergences both for the inter-parton angle  $\theta_{in} \rightarrow 0$  and for the gluon energy  $E_n \rightarrow 0$ , which are mirrored also in the structure of divergences in loop diagrams. These divergences are important for at least two reasons: firstly, they govern the typical structure of events (inducing many emissions either with low energy or at small angle with respect to hard partons); secondly, they will determine which observables can be calculated within perturbative QCD.

### 9.2.2.2. Fixed-order predictions:

Let us consider an observable  $\mathcal{O}$  that is a function  $\mathcal{O}_n(p_1, \dots, p_n)$  of the four-momenta of the  $n$  particles in an event (whether partons or hadrons). In what follows, we shall consider the cross section for events weighted with the value of the observable,  $\sigma_{\mathcal{O}}$ . As examples, if  $\mathcal{O}_n \equiv 1$  for all  $n$ , then  $\sigma_{\mathcal{O}}$  is just the total cross section; if  $\mathcal{O}_n \equiv \hat{\tau}(p_1, \dots, p_n)$  where  $\hat{\tau}$  is the value of the Thrust for that event (see Sec. 9.3.1.2), then the average value of the Thrust is  $\langle \tau \rangle = \sigma_{\mathcal{O}} / \sigma_{\text{tot}}$ ; if  $\mathcal{O}_n \equiv \delta(\tau - \hat{\tau}(p_1, \dots, p_n))$  then one gets the differential cross section as a function of the Thrust,  $\sigma_{\mathcal{O}} \equiv d\sigma/d\tau$ .

In the expressions below, we shall omit to write the non-perturbative power correction term, which for most common observables is proportional to a single power of  $\Lambda/Q$ .

**LO.** If the observable  $\mathcal{O}$  is non-zero only for events with at least  $n$  particles, then the LO QCD prediction for the weighted cross section in  $e^+e^-$  annihilation is

$$\sigma_{\mathcal{O}, LO} = \alpha_s^{n-2} (\mu_R^2) \int d\Phi_n |M_n^2(p_1, \dots, p_n)| \mathcal{O}_n(p_1, \dots, p_n), \quad (9.17)$$

where the squared tree-level matrix element,  $|M_n^2(p_1, \dots, p_n)|$ , includes relevant symmetry factors, has been summed over all subprocesses (e.g.  $e^+e^- \rightarrow q\bar{q}q\bar{q}$ ,  $e^+e^- \rightarrow q\bar{q}gg$ ) and has had all factors of  $\alpha_s$  extracted in front. In processes other than  $e^+e^-$  collisions, the

powers of the coupling are often brought inside the integrals, with the scale  $\mu_R$  chosen event by event, as a function of the event kinematics.

Other than in the simplest cases (see the review on Cross Sections in this *Review*), the matrix elements in Eq. (9.17) are usually calculated automatically with programs such as CompHEP [58], MadGraph [43], Alpgen [42], Comix/Sherpa [61], and Helac/Phegas [62]. Some of these (CompHEP, MadGraph) use formulas obtained from direct evaluations of Feynman diagrams. Others (Alpgen, Helac/Phegas and Comix/Sherpa) use methods designed to be particularly efficient at high multiplicities, such as Berends-Giele recursion [63] (see also the reviews [64,65]), which builds up amplitudes for complex processes from simpler ones.

The phase-space integration is usually carried out by Monte Carlo sampling, in order to deal with the sometimes complicated cuts that are used in corresponding experimental measurements. Because of the divergences in the matrix element, Eq. (9.16), the integral converges only if the observable vanishes for kinematic configurations in which one of the  $n$  particles is arbitrarily soft or it is collinear to another particle. As an example, the cross section for producing any configuration of  $n$  partons will lead to an infinite integral, whereas a finite result will be obtained for the cross section for producing  $n$  deposits of energy (or jets, see Sec. 9.3.1.1), each above some energy threshold and well separated from each other in angle.

LO calculations can be carried out for  $2 \rightarrow n$  processes with  $n \lesssim 6 - 10$ . The exact upper limit depends on the process, the method used to evaluate the matrix elements (recursive methods are more efficient), and the extent to which the phase-space integration can be optimized to work around the large variations in the values of the matrix elements. **NLO.** Given an observable that is non-zero starting from  $n$  particles, its prediction at NLO involves supplementing the LO result with the  $(n + 1)$ -particle tree-level matrix element ( $|M_{n+1}^2|$ ), and the interference of a  $n$ -particle tree-level and  $n$ -particle 1-loop amplitude ( $2\text{Re}(M_n M_{n,1\text{-loop}}^*)$ ),

$$\begin{aligned} \sigma_{\mathcal{O}}^{NLO} = & \sigma_{\mathcal{O}}^{LO} + \alpha_s^{n-1}(\mu_R^2) \int d\Phi_{n+1} |M_{n+1}^2(p_1, \dots, p_{n+1})| \mathcal{O}_{n+1}(p_1, \dots, p_{n+1}) \\ & + \alpha_s^{n-1}(\mu_R^2) \int d\Phi_n 2\text{Re}[M_n(p_1, \dots, p_n) \\ & M_{n,1\text{-loop}}^*(p_1, \dots, p_n)] \mathcal{O}_n(p_1, \dots, p_n) . \end{aligned} \quad (9.18)$$

Relative to LO calculations, two important issues appear in the NLO calculations. Firstly, the extra complexity of loop-calculations relative to tree-level calculations means that their automation is at a comparatively early stage (see below). Secondly, loop amplitudes are infinite in 4 dimensions, while tree-level amplitudes are finite, but their *integrals* are infinite, due to the divergences of Eq. (9.16). These two sources of infinities have the same soft and collinear origins and cancel after the integration only if the observable  $\mathcal{O}$  satisfies the property of infrared and collinear safety,

$$\begin{aligned} \mathcal{O}_{n+1}(p_1, \dots, p_s, \dots, p_n) & \rightarrow \mathcal{O}_n(p_1, \dots, p_n) & \text{if } p_s \rightarrow 0 \\ \mathcal{O}_{n+1}(p_1, \dots, p_a, p_b, \dots, p_n) & \rightarrow \mathcal{O}_n(p_1, \dots, p_a + p_b, \dots, p_n) \\ & \text{if } p_a \parallel p_b . \end{aligned} \quad (9.19)$$

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Examples of infrared safe quantities include event-shape distributions and jet cross sections (with appropriate jet algorithms, see below). Unsafe quantities include the distribution of the momentum of the hardest QCD particle (which is not conserved under collinear splitting), observables that require the complete absence of radiation in some region of phase-space (e.g. rapidity gaps or 100% isolation cuts, which are affected by soft emissions), or the particle multiplicity (affected by both soft and collinear emissions). The non-cancellation of divergences at NLO due to infrared or collinear unsafety compromises the usefulness not only of the NLO calculation, but also that of a LO calculation, since LO is only an acceptable approximation if one can prove that higher order terms are smaller. Infrared and collinear unsafety usually also imply large non-perturbative effects.

As with LO calculations, the phase-space integrals in Eq. (9.18) are usually carried out by Monte Carlo integration, so as to facilitate the study of arbitrary observables. Various methods exist to obtain numerically efficient cancellation among the different infinities. These include notably dipole [66], FKS [67] and antenna [68] subtraction.

NLO calculations have existed for a while for a wide range of  $2 \rightarrow n$  processes with  $n \leq 3$ , as reviewed in Ref. 69. Some of the corresponding codes are public, and those that provide access to multiple processes include NLOJet++ [70] for  $e^+e^-$ , DIS, and hadron-hadron processes involving just light partons in the final state, MCFM [71] for hadron-hadron processes with vector bosons and/or heavy quarks in the final state, VBFNLO for vector-boson fusion, di- and tri-boson processes [72], and the Phox family [73] for processes with photons in the final state. One forefront of NLO calculations is  $2 \rightarrow 4$  and  $2 \rightarrow 5$  processes in  $pp$  scattering (and for  $1 \rightarrow 5$  in  $e^+e^- \rightarrow \gamma/Z \rightarrow \text{hadrons}$  [74]), where recent results include  $t\bar{t}b\bar{b}$  [80,81],  $t\bar{t}+2\text{jets}$  [82] and  $b\bar{b}b\bar{b}$  [83],  $pp \rightarrow W/Z+3\text{jets}$  [75,76,77] and  $pp \rightarrow W/Z+4\text{jets}$  [78,79] as well as  $W^+W^-b\bar{b}$  [84] and  $W^+W^\pm+2\text{jets}$  [85]. A related forefront is automation: a number of the above results have been obtained with partially automated approaches. A first example of full automation applied to a large number of processes has been presented recently in Ref. 45, and a public automated code is described in Ref. 87. A number of the above calculations have made use of unitarity-type techniques [88] and powerful integrand reduction methods (notably Ref. 89), which have seen significant development over the past few years, as reviewed in Refs. 65,90.

**NNLO.** Conceptually, NNLO and NLO calculations are similar, except that one must add a further order in  $\alpha_s$ , consisting of: the squared  $(n+2)$ -parton tree-level amplitude, the interference of the  $(n+1)$ -parton tree-level and 1-loop amplitudes, the interference of the  $n$ -parton tree-level and 2-loop amplitudes, and the squared  $n$ -parton 1-loop amplitude.

Each of these elements involves large numbers of soft and collinear divergences, satisfying relations analogous to Eq. (9.16) that now involve multiple collinear or soft particles and higher loop orders (see e.g. Refs. 88,91,92). Arranging for the cancellation of the divergences after numerical Monte Carlo integration is one of the significant challenges of NNLO calculations, as is the determination of the relevant 2-loop amplitudes. At the time of writing, the processes for which fully exclusive NNLO calculations exist include the 3-jet cross section in  $e^+e^-$  collisions [93,94] (for which NNLO means  $\alpha_s^3$ ), as well as vector-boson [95,96], Higgs-boson [97,98], WH [99] and di-photon [100] production in  $pp$  and  $p\bar{p}$  collisions.

**9.2.2.3. Resummation:**

Many experimental measurements place tight constraints on emissions in the final state, for example, in  $e^+e^-$  events, that one minus the Thrust should be less than some value  $\tau \ll 1$ , or in  $pp \rightarrow Z$  events that the  $Z$ -boson transverse momentum should be much smaller than its mass,  $p_{t,Z} \ll M_Z$ . A further example is the production of heavy particles or jets near threshold (so that little energy is left over for real emissions) in DIS and  $pp$  collisions.

In such cases, the constraint vetoes a significant part of the integral over the soft and collinear divergence of Eq. (9.16). As a result, there is only a partial cancellation between real emission terms (subject to the constraint) and loop (virtual) contributions (not subject to the constraint), causing each order of  $\alpha_s$  to be accompanied by a large coefficient  $\sim L^2$ , where *e.g.*  $L = \ln \tau$  or  $L = \ln(M_Z/p_{t,Z})$ . One ends up with a perturbative series whose terms go as  $\sim (\alpha_s L^2)^n$ . It is not uncommon that  $\alpha_s L^2 \gg 1$ , so that the perturbative series converges very poorly if at all.\*\* In such cases one may carry out a “resummation,” which accounts for the dominant logarithmically enhanced terms to all orders in  $\alpha_s$ , by making use of known properties of matrix elements for multiple soft and collinear emissions, and of the all-orders properties of the divergent parts of virtual corrections, following original works such as Refs. 101–110 and also through soft-collinear effective theory [111,112] (cf. also the review in Ref. 113).

For cases with double logarithmic enhancements (two powers of logarithm per power of  $\alpha_s$ ), there are two classification schemes for resummation accuracy. Writing the cross section including the constraint as  $\sigma(L)$  and the unconstrained (total) cross section as  $\sigma_{\text{tot}}$ , the series expansion takes the form

$$\sigma(L) \simeq \sigma_{\text{tot}} \sum_{n=0}^{\infty} \sum_{k=0}^{2n} R_{nk} \alpha_s^n (\mu_R^2) L^k, \quad L \gg 1 \quad (9.20)$$

and leading log (LL) resummation means that one accounts for all terms with  $k = 2n$ , next-to-leading-log (NLL) includes additionally all terms with  $k = 2n - 1$ , *etc.* Often  $\sigma(L)$  (or its Fourier or Mellin transform) *exponentiates* †,

$$\sigma(L) \simeq \sigma_{\text{tot}} \exp \left[ \sum_{n=1}^{\infty} \sum_{k=0}^{n+1} G_{nk} \alpha_s^n (\mu_R^2) L^k \right], \quad L \gg 1, \quad (9.21)$$

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\*\* To be precise one should distinguish two causes of the divergence of perturbative series. That which interests us here is associated with the presence of a new large parameter (*e.g.* ratio of scales). Nearly all perturbative series also suffer from “renormalon” divergences  $\alpha_s^n n!$  (reviewed in Ref. 16), which however have an impact only at very high perturbative orders and have a deep connection with non-perturbative uncertainties.

† Whether or not this happens depends on the quantity being resummed. A classic example involves jet rates in  $e^+e^-$  collisions as a function of a jet-resolution parameter  $y_{\text{cut}}$ . The logarithms of  $1/y_{\text{cut}}$  exponentiate for the  $k_t$  (Durham) jet algorithm [114], but not [115] for the JADE algorithm [116] (both are discussed below in Sec. 9.3.1.1).

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where one notes the different upper limit on  $k$  ( $\leq n + 1$ ) compared to Eq. (9.20). This is a more powerful form of resummation: the  $G_{12}$  term alone reproduces the full LL series in Eq. (9.20). With the form Eq. (9.21) one still uses the nomenclature LL, but this now means that all terms with  $k = n + 1$  are included, and NLL implies all terms with  $k = n$ , *etc.*

For a large number of observables, NLL resummations are available in the sense of Eq. (9.21) (see Refs. 117–119 and references therein). NNLL has been achieved for the DY and Higgs-boson  $p_t$  distributions [120,121,122,123] (in addition the NLL ResBos program [124] is still widely used), the back-to-back energy-energy correlation in  $e^+e^-$  [125], the production of top anti-top pairs near threshold [126–128] (and references therein), high- $p_t$   $W$  and  $Z$  production [129], and an event-shape type observable known as the beam Thrust [130]. Finally, the parts believed to be dominant in the N<sup>3</sup>LL resummation are available for the Thrust variable and heavy-jet mass in  $e^+e^-$  annihilations [131,132] (confirmed for Thrust at NNLL in Ref. 133), and for Higgs- and vector-boson production near threshold [134,135] in hadron collisions (NNLL in Refs. 136,137). The inputs and methods involved in these various calculations are somewhat too diverse to discuss in detail here, so we recommend that the interested reader consult the original references for further details.

### 9.2.2.4. Fragmentation functions:

Since the parton-hadron transition is non-perturbative, it is not possible to perturbatively calculate quantities such as the energy-spectra of specific hadrons in high-energy collisions. However, one can factorize perturbative and non-perturbative contributions via the concept of fragmentation functions. These are the final-state analogue of the parton distribution functions that are used for initial-state hadrons.

It should be added that if one ignores the non-perturbative difficulties and just calculates the energy and angular spectrum of partons in perturbative QCD with some low cutoff scale  $\sim \Lambda$  (using resummation to sum large logarithms of  $\sqrt{s}/\Lambda$ ), then this reproduces many features of the corresponding hadron spectra. This is often taken to suggest that hadronization is “local” in momentum space.

Sec. 19 of this *Review* provides further information (and references) on these topics, including also the question of heavy-quark fragmentation.

### 9.2.2.5. Parton-shower Monte Carlo generators:

Parton-shower Monte Carlo (MC) event generators like PYTHIA [138–4], HERWIG [55–2], SHERPA [60], and ARIADNE [20] provide fully exclusive simulations of QCD events. Because they provide access to “hadron-level” events they are a crucial tool for all applications that involve simulating the response of detectors to QCD events. Here we give only a brief outline of how they work and refer the reader to Chap. 38 and Ref. 15 for a full overview.

The MC generation of an event involves several stages. It starts with the random generation of the kinematics and partonic channels of whatever *hard scattering process* the user has requested at some high scale  $Q_0$ . This is followed by a *parton shower*, usually based on the successive random generation of gluon emissions (or  $g \rightarrow q\bar{q}$  splittings).

Each is generated at a scale lower than the previous emission, following a (soft and collinear resummed) perturbative QCD distribution that depends on the momenta of all previous emissions. Common choices of scale for the ordering of emissions are virtuality, transverse momentum or angle. Parton showering stops at a scale of order 1 GeV, at which point a *hadronization model* is used to convert the resulting partons into hadrons. One widely-used model involves stretching a color “string” across quarks and gluons, and breaking it up into hadrons [47,148]. Another breaks each gluon into a  $q\bar{q}$  pair and then groups quarks and anti-quarks into colorless “clusters”, which then give the hadrons [55]. For  $pp$  and  $\gamma p$  processes, modeling is also needed to treat the collision between the two hadron remnants, which generates an *underlying event* (UE), usually implemented via additional  $2 \rightarrow 2$  scatterings (“multiple parton interactions”) at a scale of a few GeV, following Ref. 62.

A deficiency of the soft and collinear approximations that underlie parton showers is that they may fail to reproduce the full pattern of hard wide-angle emissions, important, for example, in many new physics searches. It is therefore common to use LO multi-parton matrix elements to generate hard high-multiplicity partonic configurations as additional starting points for the showering, supplemented with some prescription (CKKW [35], MLM [36]) for consistently merging samples with different initial multiplicities.

MCs, as described above, generate cross sections for the requested hard process that are correct at LO. For a number of processes there also exist MC implementations that are correct to NLO, using the MC@NLO [39] or POWHEG [37] prescriptions. Techniques also exist to combine NLO accuracy for a low order process, with LO accuracy for higher multiplicity processes [154,155].

### 9.2.3. Accuracy of predictions :

Estimating the accuracy of perturbative QCD predictions is not an exact science. It is often said that LO calculations are accurate to within a factor of two. This is based on experience with NLO corrections in the cases where these are available. In processes involving new partonic scattering channels at NLO and/or large ratios of scales (such as the production of high- $p_t$  jets containing  $B$ -hadrons), the NLO to LO  $K$ -factors can be substantially larger than 2.

For calculations beyond LO, a conservative approach to estimate the perturbative uncertainty is to take it to be the last known perturbative order; a more widely used method is to estimate it from the change in the prediction when varying the renormalization and factorization scales around a central value  $Q$  that is taken close to the physical scale of the process. A conventional range of variation is  $Q/2 < \mu_R, \mu_F < 2Q$ , however this should not be assumed to give uncertainty estimates of guaranteed reliability.<sup>‡‡</sup>

There does not seem to be a broad consensus on whether  $\mu_R$  and  $\mu_F$  should be kept identical or varied independently. One option is to vary them independently with

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<sup>‡‡</sup> A number of prescriptions also exist for setting the scale automatically, e.g. Refs. 156–159, eliminating uncertainties from scale variation, though not from the truncation of the perturbative series itself.

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the restriction  $\frac{1}{2}\mu_R < \mu_F < 2\mu_R$  [160]. This limits the risk of misleadingly small uncertainties due to fortuitous cancellations between the  $\mu_F$  and  $\mu_R$  dependence when both are varied together, while avoiding the appearance of large logarithms of  $\mu_R^2/\mu_F^2$  when both are varied completely independently.

Calculations that involve resummations usually have an additional source of uncertainty associated with the choice of argument of the logarithms being resummed, *e.g.*  $\ln(2\frac{p_{t,Z}}{M_Z})$  as opposed to  $\ln(\frac{1}{2}\frac{p_{t,Z}}{M_Z})$ . In addition to varying renormalization and factorization scales, it is therefore also advisable to vary the argument of the logarithm by a factor of two in either direction with respect to the “natural” argument.

The accuracy of QCD predictions is limited also by non-perturbative corrections, which typically scale as a power of  $\Lambda/Q$ . For measurements that are directly sensitive to the structure of the hadronic final state the corrections are usually linear in  $\Lambda/Q$ . The non-perturbative corrections are further enhanced in processes with a significant underlying event (*i.e.* in  $pp$  and  $p\bar{p}$  collisions) and in cases where the perturbative cross sections fall steeply as a function of  $p_t$  or some other kinematic variable.

Non-perturbative corrections are commonly estimated from the difference between Monte Carlo events at the parton level and after hadronization. An issue to be aware of with this procedure is that “parton level” is not a uniquely defined concept. For example, in an event generator it depends on a (somewhat arbitrary and tunable) internal cutoff scale that separates the parton showering from the hadronization. In contrast no such cutoff scale exists in a NLO or NNLO partonic calculation. For this reason there are widespread reservations as to the appropriateness of deriving hadronization corrections from a Monte Carlo program and then applying them to NLO or NNLO prediction. There exist alternative methods for estimating hadronization corrections, which attempt to analytically deduce non-perturbative effects in one observable based on measurements of other observables (see the reviews [16,161]). While they directly address the problem of different possible definitions of parton level, it should also be said that they are far less flexible than Monte Carlo programs and not always able to provide equally good descriptions of the data.

### 9.3. Experimental QCD

Since we are not able to directly measure partons (quarks or gluons), but only hadrons and their decay products, a central issue for every experimental test of QCD is establishing a correspondence between observables obtained at the partonic and the hadronic level. The only theoretically sound correspondence is achieved by means of *infrared and collinear safe* quantities, which allow one to obtain finite predictions at any order of perturbative QCD.

As stated above, the simplest case of infrared and collinear safe observables are total cross sections. More generally, when measuring fully inclusive observables, the final state is not analyzed at all regarding its (topological, kinematical) structure or its composition. Basically the relevant information consists in the rate of a process ending up in a partonic or hadronic final state. In  $e^+e^-$  annihilation, widely used examples are the ratios of partial widths or branching ratios for the electroweak decay of particles into hadrons



or leptons, such as  $Z$  or  $\tau$  decays, (cf. Sec. 9.2.1). Such ratios are often favored over absolute cross sections or partial widths because of large cancellations of experimental and theoretical systematic uncertainties. The strong suppression of non-perturbative effects,  $\mathcal{O}(\Lambda^4/Q^4)$ , is one of the attractive features of such observables, however, at the same time the sensitivity to radiative QCD corrections is small, which for example affects the statistical uncertainty when using them for the determination of the strong coupling constant. In the case of  $\tau$  decays not only the hadronic branching ratio is of interest, but also moments of the spectral functions of hadronic tau decays, which sample different parts of the decay spectrum and thus provide additional information. Other examples of fully inclusive observables are structure functions (and related sum rules) in DIS. These are extensively discussed in Sec. 18 of this *Review*.

On the other hand, often the structure or composition of the final state are analyzed and cross sections differential in one or more variables characterizing this structure are of interest. Examples are jet rates, jet substructure, event shapes or transverse momentum distributions of jets or vector bosons in hadron collisions. The case of fragmentation functions, *i.e.* the measurement of hadron production as a function of the hadron momentum relative to some hard scattering scale, is discussed in Sec. 19 of this *Review*.

It is worth mentioning that, besides the correspondence between the parton and hadron level, also a correspondence between the hadron level and the actually measured quantities in the detector has to be established. The simplest examples are corrections for finite experimental acceptance and efficiencies. Whereas acceptance corrections essentially are of theoretical nature, since they involve extrapolations from the measurable (partial) to the full phase space, other corrections such as for efficiency, resolution and response, are of experimental nature. For example, measurements of differential cross sections such as jet rates require corrections in order to relate, *e.g.* the energy deposits in a calorimeter to the jets at the hadron level. Typically detector simulations and/or data driven methods are used in order to obtain these corrections. Care should be taken here in order to have a clear separation between the parton-to-hadron level and hadron-to-detector level corrections. Finally, for the sake of an easy comparison to the results of other experiments and/or theoretical calculations, it is suggested to provide, whenever possible, measurements corrected for detector effects and/or all necessary information related to the detector response (*e.g.* the detector response matrix).

### 9.3.1. Hadronic final-state observables :

#### 9.3.1.1. Jets:

In hard interactions, final-state partons and hadrons appear predominantly in collimated bunches. These bunches are generically called *jets*. To a first approximation, a jet can be thought of as a hard parton that has undergone soft and collinear showering and then hadronization. Jets are used both for testing our understanding and predictions of high-energy QCD processes, and also for identifying the hard partonic structure of decays of massive particles like top quarks.

In order to map observed hadrons onto a set of jets, one uses a *jet definition*. The mapping involves explicit choices: for example when a gluon is radiated from a quark, for what range of kinematics should the gluon be part of the quark jet, or instead form

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a separate jet? Good jet definitions are infrared and collinear safe, simple to use in theoretical and experimental contexts, applicable to any type of inputs (parton or hadron momenta, charged particle tracks, and/or energy deposits in the detectors) and lead to jets that are not too sensitive to non-perturbative effects. An extensive treatment of the topic of jet definitions is given in Ref. 162 (for  $e^+e^-$  collisions) and Refs. 163, 164 (for  $pp$  or  $p\bar{p}$  collisions). Here we briefly review the two main classes: cone algorithms, extensively used at older hadron colliders, and sequential recombination algorithms, more widespread in  $e^+e^-$  and  $ep$  colliders and at the LHC.

Very generically, most (iterative) cone algorithms start with some seed particle  $i$ , sum the momenta of all particles  $j$  within a cone of opening-angle  $R$ , typically defined in terms of (pseudo-)rapidity and azimuthal angle. They then take the direction of this sum as a new seed and repeat until the cone is stable, and call the contents of the resulting stable cone a jet if its transverse momentum is above some threshold  $p_{t,\min}$ . The parameters  $R$  and  $p_{t,\min}$  should be chosen according to the needs of a given analysis.

There are many variants of cone algorithm, and they differ in the set of seeds they use and the manner in which they ensure a one-to-one mapping of particles to jets, given that two stable cones may share particles (“overlap”). The use of seed particles is a problem w.r.t. infrared and collinear safety, and seeded algorithms are generally not compatible with higher-order (or sometimes even leading-order) QCD calculations, especially in multi-jet contexts, as well as potentially subject to large non-perturbative corrections and instabilities. Seeded algorithms (JetCLU, MidPoint, and various other experiment-specific iterative cone algorithms) are therefore to be deprecated. A modern alternative is to use a seedless variant, SIScone [165].

Sequential recombination algorithms at hadron colliders (and in DIS) are characterized by a distance  $d_{ij} = \min(k_{t,i}^{2p}, k_{t,j}^{2p})\Delta_{ij}^2/R^2$  between all pairs of particles  $i, j$ , where  $\Delta_{ij}$  is their distance in the rapidity-azimuthal plane,  $k_{t,i}$  is the transverse momentum w.r.t. the incoming beams, and  $R$  is a free parameter. They also involve a “beam” distance  $d_{iB} = k_{t,i}^{2p}$ . One identifies the smallest of all the  $d_{ij}$  and  $d_{iB}$ , and if it is a  $d_{ij}$ , then  $i$  and  $j$  are merged into a new pseudo-particle (with some prescription, a recombination scheme, for the definition of the merged four-momentum). If the smallest distance is a  $d_{iB}$ , then  $i$  is removed from the list of particles and called a jet. As with cone algorithms, one usually considers only jets above some transverse-momentum threshold  $p_{t,\min}$ . The parameter  $p$  determines the kind of algorithm:  $p = 1$  corresponds to the (*inclusive*-) $k_t$  algorithm [114,166,167],  $p = 0$  defines the *Cambridge-Aachen* algorithm [168,169], while for  $p = -1$  we have the *anti*- $k_t$  algorithm [170]. All these variants are infrared and collinear safe to all orders of perturbation theory. Whereas the former two lead to irregularly shaped jet boundaries, the latter results in cone-like boundaries. The *anti*- $k_t$  algorithm has become the de-facto standard for the LHC experiments.

In  $e^+e^-$  annihilations the  $k_t$  algorithm [114] uses  $y_{ij} = 2 \min(E_i^2, E_j^2)(1 - \cos \theta_{ij})/Q^2$  as distance measure and repeatedly merges the pair with smallest  $y_{ij}$ , until all  $y_{ij}$  distances are above some threshold  $y_{\text{cut}}$ , the jet resolution parameter. The (pseudo)-particles that remain at this point are called the jets. Here it is  $y_{\text{cut}}$  (rather than  $R$  and  $p_{t,\min}$ ) that should be chosen according to the needs of the analysis. As mentioned above, the

$k_t$  algorithm has the property that logarithms  $\ln(1/y_{\text{cut}})$  exponentiate in resummation calculations. This is one reason why it is preferred over the earlier JADE algorithm [116], which uses the distance measure  $y_{ij} = 2 E_i E_j (1 - \cos \theta_{ij})/Q^2$ .

Efficient implementations of the above algorithms are available through the *FastJet* package [171], which is also packaged within *SpartyJet* [172].

### 9.3.1.2. Event Shapes:

Event-shape variables are functions of the four momenta in the hadronic final state that characterize the topology of an event's energy flow. They are sensitive to QCD radiation (and correspondingly to the strong coupling) insofar as gluon emission changes the shape of the energy flow.

The classic example of an event shape is the *Thrust* [173,174] in  $e^+e^-$  annihilations, defined as

$$\hat{\tau} = \max_{\vec{n}_\tau} \frac{\sum_i |\vec{p}_i \cdot \vec{n}_\tau|}{\sum_i |\vec{p}_i|}, \quad (9.22)$$

where  $\vec{p}_i$  are the momenta of the particles or the jets in the final-state and the maximum is obtained for the Thrust axis  $\vec{n}_\tau$ . In the Born limit of the production of a perfect back-to-back  $q\bar{q}$  pair the limit  $\hat{\tau} \rightarrow 1$  is obtained, whereas a perfectly symmetric many-particle configuration leads to  $\hat{\tau} \rightarrow 1/2$ . Further event shapes of similar nature have been defined and extensively measured at LEP and at HERA, and for their definitions and reviews we refer to Refs. 3,4,161,175,176. Phenomenological discussions of event shapes at hadron colliders can be found in Refs. 177–179. Very recently, measurements of hadronic event-shape distributions have been published by CDF [180] and CMS [181].

Event shapes are used for many purposes. These include measuring the strong coupling, tuning the parameters of Monte Carlo programs, investigating analytical models of hadronization and distinguishing QCD events from events that might involve decays of new particles (giving event-shape values closer to the spherical limit).

### 9.3.1.3. Jet substructure, quark vs. gluon jets:

Jet substructure, which can be resolved by finding subjets or by measuring jet shapes, is sensitive to the details of QCD radiation in the shower development inside a jet and has been extensively used to study differences in the properties of quark and gluon induced jets, strongly related to their different color charges. In general there is clear experimental evidence that gluon jets are “broader” and have a softer particle spectrum than (light-) quark jets, whereas b-quark jets are similar to gluon jets. As an example of an observable, the jet shape  $\Psi(r/R)$  is the fractional transverse momentum contained within a sub-cone of cone-size  $r$  for jets of cone-size  $R$ . It is sensitive to the relative fractions of quark and gluon jets in an inclusive jet sample and receives contributions from soft-gluon initial-state radiation and beam remnant-remnant interactions. Therefore, it has been widely employed for validation and tuning of Monte Carlo models. CDF has measured the jet shape  $\Psi(r/R)$  for an inclusive jet sample [182] as well as for b-jets [183]. Similar measurements in photo-production and DIS at HERA have been reported in Refs. 184–186. First measurements at the LHC have been presented by ATLAS [187]. Further

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discussions, references and recent summaries can be found in Refs. 176, 188 and Sec. 4 of Ref. 189.

The use of jet substructure has also been suggested in order to distinguish QCD jets from jets that originate from hadronic decays of boosted massive particles (high- $p_t$  electroweak bosons, top quarks and hypothesized new particles). For reviews and detailed references, see Ref. 189 and sec. 5.3 of Ref. 163.

### 9.3.2. State of the art QCD measurements at colliders :

There exists an enormous wealth of data on QCD-related measurements in  $e^+e^-$ ,  $ep$ ,  $pp$ , and  $p\bar{p}$  collisions, to which a short overview like this would not be able to do any justice. Extensive reviews of the subject have been published in Refs. 175, 176 for  $e^+e^-$  colliders, whereas for hadron colliders comprehensive overviews are given in Refs. 164, 190, and recent summaries can be found in, *e.g.* Refs. 191–194.

Below we concentrate our discussion on measurements that are most sensitive to hard QCD processes, in particular jet production.

**9.3.2.1.  $e^+e^-$  colliders:** Analyses of jet production in  $e^+e^-$  collisions are mostly based on JADE data at center-of-mass energies between 14 and 44 GeV, as well as on LEP data at the  $Z$  resonance and up to 209 GeV. They cover the measurements of (differential or exclusive) jet rates (with multiplicities typically up to 4, 5 or 6 jets), the study of 3-jet events and particle production between the jets as a tool for testing hadronization models, as well as 4-jet production and angular correlations in 4-jet events. The latter are useful for measurements of the strong coupling constant and putting constraints on the QCD color factors, thus probing the non-abelian nature of QCD. There have also been extensive measurements of event shapes. The tuning of parton shower MC models, typically matched to matrix elements for 3-jet production, has led to good descriptions of the available, highly precise data. Especially for the large LEP data sample at the  $Z$  peak, the statistical errors are mostly negligible and the experimental systematic uncertainties are at the per-cent level or even below. These are usually dominated by the uncertainties related to the MC model dependence of the efficiency and acceptance corrections (often referred to as “detector corrections”).

**9.3.2.2. DIS and photoproduction:** Multi-jet production in  $ep$  collisions at HERA, both in the DIS and photoproduction regime, allows for tests of QCD factorization (one initial-state proton and its associated PDF versus the hard scattering which leads to high- $p_t$  jets) and NLO calculations which exist for 2- and 3-jet final states. Sensitivity is also obtained to the product of the coupling constant and the gluon PDF. By now experimental uncertainties of the order of 5 – 10% have been achieved, mostly dominated by jet energy scale uncertainties, whereas statistical errors are negligible to a large extent. For comparison to theoretical predictions, at large jet  $p_t$  the PDF uncertainty dominates the theoretical error (typically of order 5 - 10%, in some regions of phase-space up to 20%), therefore jet observables become useful inputs for PDF fits. In general, for  $Q^2$  above  $\sim 100 \text{ GeV}^2$  the data are well described by NLO matrix element calculations, combined with DGLAP evolution equations. Results at lower values ( $Q^2 < 100 \text{ GeV}^2$ ) point to the necessity of including NNLO effects. Also, at low values of  $Q^2$  and  $x$ , in

particular for large jet pseudo-rapidities, there are indications for the need of BFKL-type evolution, though the predictions for such schemes are still limited. In the case of photoproduction, the data-theory comparisons are hampered by the uncertainties related to the photon PDF.

A few examples of recent measurements can be found in Refs. 195–200 for DIS and in Refs. 201–205 for photoproduction.

**9.3.2.3. Hadron colliders:** Jet measurements at the TEVATRON have been published for data samples up to  $\sim 2\text{fb}^{-1}$ . Also, first results from the LHC have become available, for a center-of-mass energy of 7 TeV and sample sizes of up to  $\sim 36\text{pb}^{-1}$ . Among the most important cross sections measured is the inclusive jet production as a function of the jet transverse energy ( $E_t$ ) or the jet transverse momentum ( $p_t$ ), for several rapidity regions and for  $p_t$  up to 700 GeV at the TEVATRON and  $\sim 1$  TeV at the LHC. The TEVATRON experiments have measurements based on the infrared- and collinear-safe  $k_t$  algorithm in addition to the more widely used Midpoint and JetCLU algorithms of the past, whereas the LHC experiments focus on the *anti- $k_t$*  algorithm. Results by the CDF and D0 collaborations can be found in Refs. 206–208, whereas first measurements of ATLAS and CMS have been published in Refs. 209 and 210, respectively. In general we observe a good description of the data by the NLO QCD predictions. The experimental systematic uncertainties are dominated by the jet energy scale error, by now quoted to be in the range of 1 to 3% and thus leading to uncertainties of 10 to 60% on the cross section, increasing with  $p_t$ . The PDF uncertainties dominate the theoretical error. In fact, inclusive jet data are important inputs to global PDF fits, in particular for constraining the high- $x$  gluon PDF.

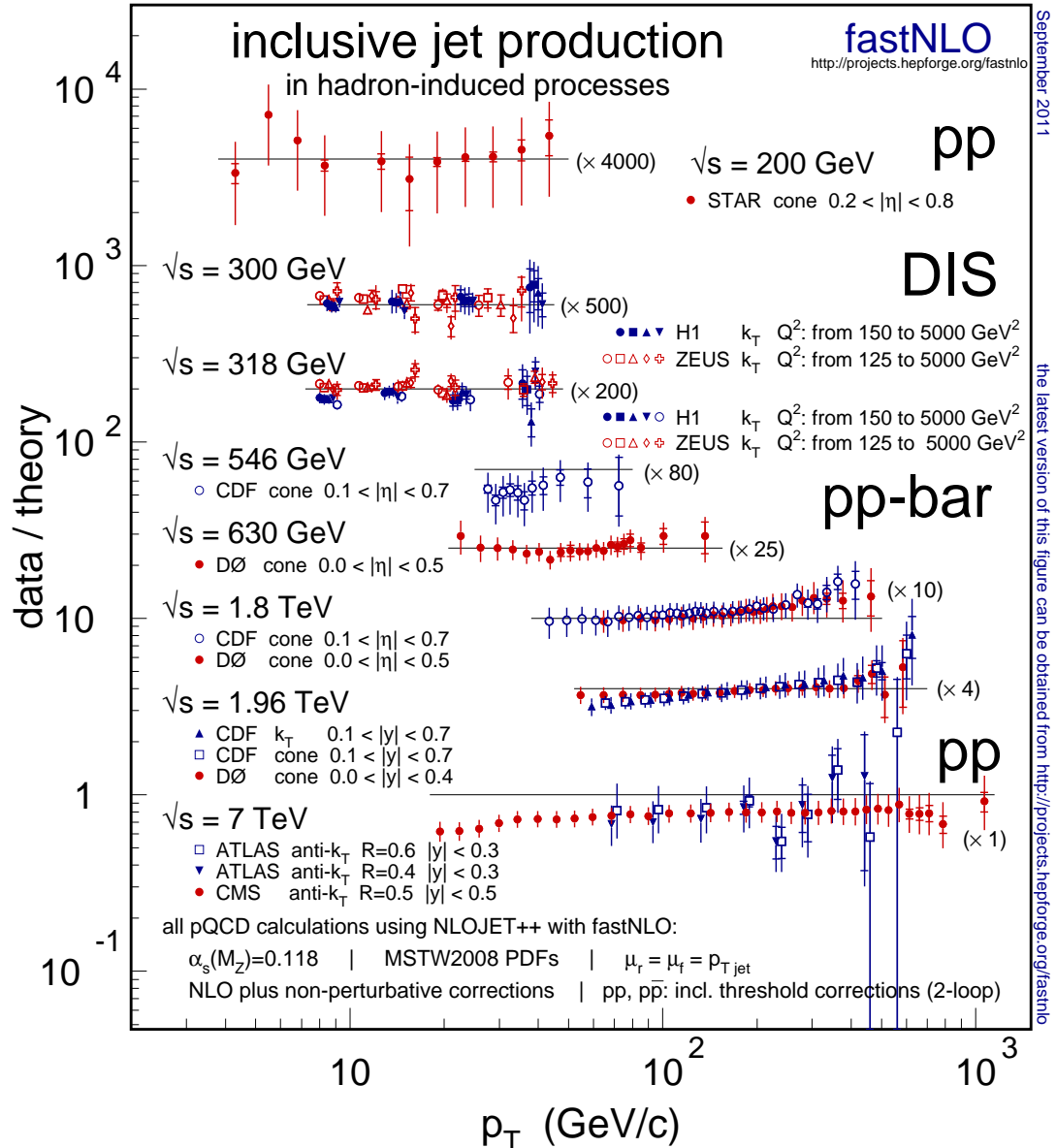
A rather comprehensive summary, comparing NLO QCD predictions to data for inclusive jet production in DIS,  $pp$ , and  $p\bar{p}$  collisions, is given in Ref. 211 and reproduced here in Fig. 9.1.

Dijet events are analyzed in terms of their invariant mass and angular distributions, which allow one to put stringent limits on deviations from the Standard Model, such as quark compositeness (some recent examples can be found in Refs. 212–217). Furthermore, dijet azimuthal correlations between the two leading jets, normalized to the total dijet cross section, are an extremely valuable tool for studying the spectrum of gluon radiation in the event. For example, results from the TEVATRON [218] and the LHC [219,220] show that the LO (non-trivial) prediction for this observable, with at most three partons in the final state, is not able to describe the data for an azimuthal separation below  $2\pi/3$ , where NLO contributions (with 4 partons) restore the agreement with data. In addition, this observable can be employed to tune Monte Carlo predictions of soft gluon radiation. Beyond dijet final states, recently measurements of the production of three or more jets have been performed [221–223], as a means of testing perturbative QCD predictions, tuning MC models, constraining PDFs or determining the strong coupling constant.

Similarly important tests of QCD arise from measurements of vector boson (photon,  $W$ ,  $Z$ ) production together with jets. A recent analysis of photon+jet production by D0 [224] indicates that NLO calculations, combined with modern PDF sets, are unable to

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describe the shape of the photon  $p_t$  across the entire measured range, showing the need for an improved and consistent theoretical description of this process.



**Figure 9.1:** A compilation of data-over-theory ratios for inclusive jet cross sections as a function of jet transverse momentum ( $p_T$ ), measured in different hadron-induced processes at different center-of-mass energies; from Ref. 211. The various ratios are scaled by arbitrary numbers (indicated between parentheses) for better readability of the plot. The theoretical predictions have been obtained at NLO accuracy, for parameter choices (coupling constant, PDFs, renormalization, and factorization scales) as indicated at the bottom of the figure.

In the case of  $Z$ +jets, the  $Z$  momentum can be precisely reconstructed using the leptons, allowing for a precise determination of the  $Z$   $p_t$  distribution, which is sensitive to QCD radiation both at high and low scales and thus probes perturbative as well as non-perturbative effects. For example, a recent D0 result [225] quotes experimental statistical and systematic uncertainties of the order of 10%, increasing up to 20% in the lowest momentum range. The data are compared to predictions from NLO QCD and from different Monte Carlo models, where, for example, LO matrix elements for up to three partons are matched to a parton shower. Whereas the total cross section is underestimated, the shape is well reproduced over a large phase-space region. Similar conclusions are drawn from further results on  $Z$  (or  $W$ ) plus jets production, both from the TEVATRON [226–231] and the LHC [232,233]. A very important recent development is the completion of NLO calculations for vector boson plus 3jet [75–77] and 4jet production [78,79], which is relevant also for background estimations in the searches for new physics. This type of process is an example where jets need to be found with an infrared and collinear safe jet algorithm in order to obtain finite NLO predictions. This would not be possible with algorithms such as Midpoint or JetCLU, used in analyses at the TEVATRON [228,231]. There the measurements are compared to the NLO QCD prediction obtained with SIScone as jet algorithm. Besides this inconsistency, the agreement appears to be reasonably good.

Finally, examples of recent TEVATRON measurements of heavy quark ( $b$ ,  $c$ ) jet production, inclusive or in association with vector bosons, can be found in Refs. 234–240. Also, first results for vector boson production in association with  $b$ -jets have been obtained at the LHC [241,242]. It is worth noting that for  $W+b$  production there is some tension between the measurements and the NLO predictions, in particular in the case of the CDF result [239].

### 9.3.3. Tests of the non-abelian nature of QCD :

QCD is a gauge theory with  $SU(3)$  as underlying gauge group. For a general gauge theory with a simple Lie group, the couplings of the fermion fields to the gauge fields and the self-interactions in the non-abelian case are determined by the coupling constant and Casimir operators of the gauge group, as introduced in Sec. 9.1. Measuring the eigenvalues of these operators, called color factors, probes the underlying structure of the theory in a gauge invariant way and provides evidence of the gluon self-interactions. Typically, cross sections can be expressed as functions of the color factors, for example  $\sigma = f(\alpha_s C_F, C_A/C_F, n_f T_R/C_F)$ . Sensitivity at leading order in perturbation theory can be achieved by measuring angular correlations in 4-jet events in  $e^+e^-$  annihilation or 3-jet events in DIS. Some sensitivity, although only at NLO, is also obtained from event-shape distributions. Scaling violations of fragmentation functions and the different subjet structure in quark and gluon induced jets also give access to these color factors. In order to extract absolute values, *e.g.* for  $C_F$  and  $C_A$ , certain assumptions have to be made for other parameters, such as  $T_R, n_f$  or  $\alpha_s$ , since typically only combinations (ratios, products) of all the relevant parameters appear in the perturbative prediction. A recent compilation of results [176] quotes world average values of  $C_A = 2.89 \pm 0.03(\text{stat}) \pm 0.21(\text{syst})$  and  $C_F = 1.30 \pm 0.01(\text{stat}) \pm 0.09(\text{syst})$ , with a correlation coefficient of 82%. These results are in perfect agreement with the

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expectations from SU(3) of  $C_A = 3$  and  $C_F = 4/3$ . An overview of the history and the current status of tests of Asymptotic Freedom, closely related to the non-abelian nature of QCD, can be found in Ref. 243.

### 9.3.4. Measurements of the strong coupling constant :

If the quark masses are fixed, there is only one free parameter in the QCD Lagrangian, the strong coupling constant  $\alpha_s$ . The coupling constant in itself is not a physical observable, but rather a quantity defined in the context of perturbation theory, which enters predictions for experimentally measurable observables, such as  $R$  in Eq. (9.7).

Many experimental observables are used to determine  $\alpha_s$ . Considerations in such determinations include:

- The observable's sensitivity to  $\alpha_s$  as compared to the experimental precision. For example, for the  $e^+e^-$  cross section to hadrons (cf.  $R$  in Sec. 9.2.1), QCD effects are only a small correction, since the perturbative series starts at order  $\alpha_s^0$ ; 3-jet production or event shapes in  $e^+e^-$  annihilations are directly sensitive to  $\alpha_s$  since they start at order  $\alpha_s$ ; the hadronic decay width of heavy quarkonia,  $\Gamma(\Upsilon \rightarrow \text{hadrons})$ , is very sensitive to  $\alpha_s$  since its leading order term is  $\propto \alpha_s^3$ .
- The accuracy of the perturbative prediction, or equivalently of the relation between  $\alpha_s$  and the value of the observable. The minimal requirement is generally considered to be an NLO prediction. Some observables are predicted to NNLO (many inclusive observables, 3-jet rates and event shapes in  $e^+e^-$  collisions) or even N<sup>3</sup>LO ( $e^+e^-$  hadronic cross section and  $\tau$  branching fraction to hadrons). In certain cases, fixed-order predictions are supplemented with resummation. The precise magnitude of theory uncertainties is usually estimated as discussed in Sec. 9.2.3.
- The size of uncontrolled non-perturbative effects (except for lattice-based determinations of  $\alpha_s$ ). Sufficiently inclusive quantities, like the  $e^+e^-$  cross section to hadrons, have small non-perturbative uncertainties  $\sim \Lambda^4/Q^4$ . Others, such as event-shape distributions, have uncertainties  $\sim \Lambda/Q$ .
- The scale at which the measurement is performed. An uncertainty  $\delta$  on a measurement of  $\alpha_s(Q^2)$ , at a scale  $Q$ , translates to an uncertainty  $\delta' = (\alpha_s^2(M_Z^2)/\alpha_s^2(Q^2)) \cdot \delta$  on  $\alpha_s(M_Z^2)$ . For example, this enhances the already important impact of precise low- $Q$  measurements, such as from  $\tau$  decays, in combinations performed at the  $M_Z$  scale.

In this review, we update the measurements of  $\alpha_s$  summarized in the 2009 review, which was based on an analysis by Bethke [244], and we extract a new world average value of  $\alpha_s(M_Z^2)$  from the most significant and complete results available today<sup>‡</sup>.

While in general we follow the same selection strategy and summary procedure as applied in the 2009 review, here we restrict the selection of results from which to calculate the world average value of  $\alpha_s(M_Z^2)$  to those which are

- published in a peer-reviewed journal

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<sup>‡</sup> The time evolution of  $\alpha_s$  combinations can be followed by consulting Refs. 243, 245 as well as earlier editions of this *Review*.



- based on the most complete perturbative QCD predictions, i.e. to those using NNLO or higher order expansions.

While this excludes e.g. results from jet production in DIS at HERA and at the Tevatron, as well as those from heavy quarkonia decays for which calculations are available in NLO only, these NLO results will nevertheless be listed and cited in this review as they are important ingredients for the experimental evidence of the energy dependence of  $\alpha_s$ , i.e. for Asymptotic Freedom, one of the key features of QCD.

In addition, here we add an intermediate step of pre-averaging results within certain sub-fields like  $e^+e^-$ -annihilation, DIS and hadronic  $\tau$ -decays, and calculate the overall world average from those pre-averages rather than from individual measurements. This is done because in a number of sub-fields one observes that different determinations of the strong coupling from substantially similar datasets lead to values of  $\alpha_s$  that are only marginally compatible with each other, or with the final world average value, which presumably is a reflection of the challenges of evaluating systematic uncertainties. In such cases, a pre-average value will be determined, with a symmetric, overall error that encompasses the central values of all individual determinations.

#### *Hadronic $\tau$ decays*

Several re-analyses of the hadronic  $\tau$  decay width [17,246–250], based on the new N<sup>3</sup>LO predictions [17], have been performed, with different approaches towards the detailed treatment of the perturbative (fixed-order or contour-improved perturbative expansions) and non-perturbative contributions. We also include the result from  $\tau$  decay and lifetime measurements, obtained in Sec. *Electroweak Model and constraints on New Physics* of this *Review*, which amounts, if converted to the  $\tau$ -mass scale and for  $n_f = 3$  quark flavours, to  $\alpha_s(M_\tau) = 0.327^{+0.019}_{-0.016}$ . This result and the one from Baikov et al. [17] include both fixed-order and contour-improved perturbation, while the others adhere to either one or the other of the two. All these results are summarized in Fig. 9.2(a). We note that there are more studies of  $\alpha_s$  from  $\tau$ -decays, [251–254], which are not yet available as peer-reviewed publications but which are compatible with the overall picture. Another recent study [255] argues that an improved treatment of non-perturbative effects results in values of  $\alpha_s$  which are systematically lower than those discussed above. Results using the same analysis framework, but employing an updated version of the OPAL tau spectral function data are reported in Ref. 256, which at the time of writing was as yet unpublished.

We determine the pre-average result from  $\tau$ -decays, to be used for calculating the final world average of  $\alpha_s(M_Z^2)$ , using the simple method defined above, as  $\alpha_s(M_\tau^2) = 0.330 \pm 0.014$ , which spans the range of central values obtained by the different groups. This value of  $\alpha_s(M_\tau^2)$  corresponds, when evolved to the scale of the  $Z$ -boson, using the QCD 4-loop beta-function plus 3-loop matching at the charm- and the bottom-quark masses (see Sec. *Quark Masses* in this *Review*), to  $\alpha_s(M_Z^2) = 0.1197 \pm 0.0016$ , unchanged from its value in the 2009 review.

#### *Lattice QCD*

There are several recent results on  $\alpha_s$  from lattice QCD, see also Sec. *Lattice QCD* in this *Review*. The HPQCD collaboration [257] computes Wilson loops and similar

short-distance quantities with lattice QCD and analyzes them with NNLO perturbative QCD. This yields a value for  $\alpha_s$ , but the lattice scale must be related to a physical energy/momentum scale. This is achieved with the  $\Upsilon'$ - $\Upsilon$  mass difference, however, many other quantities could be used as well [258]. HPQCD obtains  $\alpha_s(M_Z^2) = 0.1184 \pm 0.0006$ , where the uncertainty includes effects from truncating perturbation theory, finite lattice spacing and extrapolation of lattice data. An independent perturbative analysis of a subset of the same lattice-QCD data yields  $\alpha_s(M_Z^2) = 0.1192 \pm 0.0011$  [259]. Using another, independent methodology, the current-current correlator method, HPQCD obtains  $\alpha_s(M_Z^2) = 0.1183 \pm 0.0007$  [257]. The analysis of Ref. 89, which avoids the staggered fermion treatment of Ref. 257, finds  $\alpha_s(M_Z^2) = 0.1205 \pm 0.0008 \pm 0.0005^{+0.0000}_{-0.0017}$ , where the first uncertainty is statistical and the others are from systematics. Since this approach uses a different discretization of lattice fermions and a different general methodology, it provides an independent cross check of other lattice extractions of  $\alpha_s$ . Finally, the JLQCD collaboration - in an analysis of Adler functions - obtains  $\alpha_s(M_Z^2) = 0.1181 \pm 0.0003^{+0.0014}_{-0.0012}$  [261]. A very recent but unpublished study of the ETM collaboration [262] used lattice data with u, d, s and c quarks in the sea, obtaining results which are compatible with those quoted above.

The published lattice results are summarized in Fig. 9.2(b). Since they are compatible with each other, we calculate a pre-average of lattice results using the same method as applied to determine the final world average value of the strong coupling, i.e. calculate a weighted average and a (correlated) error such that the overall  $\chi^2$  equals unity per degree of freedom - rather than using the simple method as applied in the case of  $\tau$  decays. This gives  $\alpha_s(M_Z^2) = 0.1185 \pm 0.0007$  which we take as result from the sub-field of lattice determinations.

#### *Deep inelastic lepton-nucleon scattering (DIS)*

Studies of DIS final states have led to a number of precise determinations of  $\alpha_s$ : A combination [263] of precision measurements at HERA, based on NLO fits to inclusive jet cross sections in neutral current DIS at high  $Q^2$ , quotes a combined result of  $\alpha_s(M_Z^2) = 0.1198 \pm 0.0032$ , which includes a theoretical uncertainty of  $\pm 0.0026$ . A combined analysis of non-singlet structure functions from DIS [264], based on QCD predictions up to N<sup>3</sup>LO in some of its parts, gave  $\alpha_s(M_Z^2) = 0.1142 \pm 0.0023$ , including a theoretical error of  $\pm 0.0008$  (BBG). Further studies of singlet and non-singlet structure functions, based on NNLO predictions, resulted in  $\alpha_s(M_Z^2) = 0.1129 \pm 0.0014$  [265] (ABKM; updated in a recent unpublished note [266]) and in  $\alpha_s(M_Z^2) = 0.1158 \pm 0.0035$  [267] (JR). The MSTW group [268], also including data on jet production at the Tevatron, obtains, at NNLO<sup>##</sup>,  $\alpha_s(M_Z^2) = 0.1171 \pm 0.0024$ . Most recently, the NNPDF group [269] has presented a result,  $\alpha_s(M_Z^2) = 0.1173 \pm 0.0011$ . which is in line with the one from the MSTW group.

Summarizing these results from world data on structure functions, applying the same method as in the case of summarizing results from  $\tau$  decays, leads to a pre-average value of  $\alpha_s(M_Z^2) = 0.1151 \pm 0.0022$  (see Fig. 9.2(c)).

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<sup>##</sup> Note that for jet production at the hadron collider, only NLO predictions are available, while for the structure functions full NNLO was utilized.

We note that criticism has been expressed on some of the above extractions. Among the issues raised, we mention the neglect of singlet contributions at  $x \geq 0.3$  in pure non-singlet fits [270], the impact and detailed treatment of particular classes of data in the fits [270,271] and possible biases due to insufficiently flexible parametrizations of the PDFs [272].

#### *Heavy quarkonia decays*

The most recent extraction of the strong coupling constant from an analysis of radiative  $\Upsilon$  decays [273] resulted in  $\alpha_s(M_Z) = 0.119^{+0.006}_{-0.005}$ . This determination is based on QCD in NLO only, so it will not be considered for the final extraction of the world average value of  $\alpha_s$ ; it is, however, an important ingredient for the demonstration of Asymptotic Freedom as given in Fig. 9.4.

#### *Hadronic final states of $e^+e^-$ annihilations*

Re-analyses of event shapes in  $e^+e^-$ -annihilation, measured at the  $Z$  peak and LEP2 energies up to 209 GeV, using NNLO predictions matched to NLL resummation, resulted in  $\alpha_s(M_Z^2) = 0.1224 \pm 0.0039$  [274], with a dominant theoretical uncertainty of 0.0035, and in  $\alpha_s(M_Z^2) = 0.1189 \pm 0.0043$  [275]. Similarly, an analysis of JADE data [276] at center-of-mass energies between 14 and 46 GeV gives  $\alpha_s(M_Z^2) = 0.1172 \pm 0.0051$ , with contributions from hadronization model (perturbative QCD) uncertainties of 0.0035 (0.0030). A precise determination of  $\alpha_s$  from 3-jet production alone, in NNLO, resulted in  $\alpha_s(M_Z^2) = 0.1175 \pm 0.0025$  [277]. Computation of the NLO corrections to 5-jet production and comparison to the measured 5-jet rates at LEP [74] gave  $\alpha_s(M_Z^2) = 0.1156^{+0.0041}_{-0.0034}$ . More recently, a study using the world data of Thrust distributions and soft-collinear effective theory, including fixed order NNLO, gave  $\alpha_s(M_Z^2) = 0.1135 \pm 0.0010$  [278]. We note that there is criticism on both classes of  $\alpha_s$  extractions just described: those based on corrections of non-perturbative hadronisation effects using QCD-inspired Monte Carlo generators (since the parton level of a Monte Carlo is not defined in a manner equivalent to that of a fixed-order calculation), as well as the studies based on effective field theory, as their systematics have not yet been verified e.g. by using observables other than Thrust.

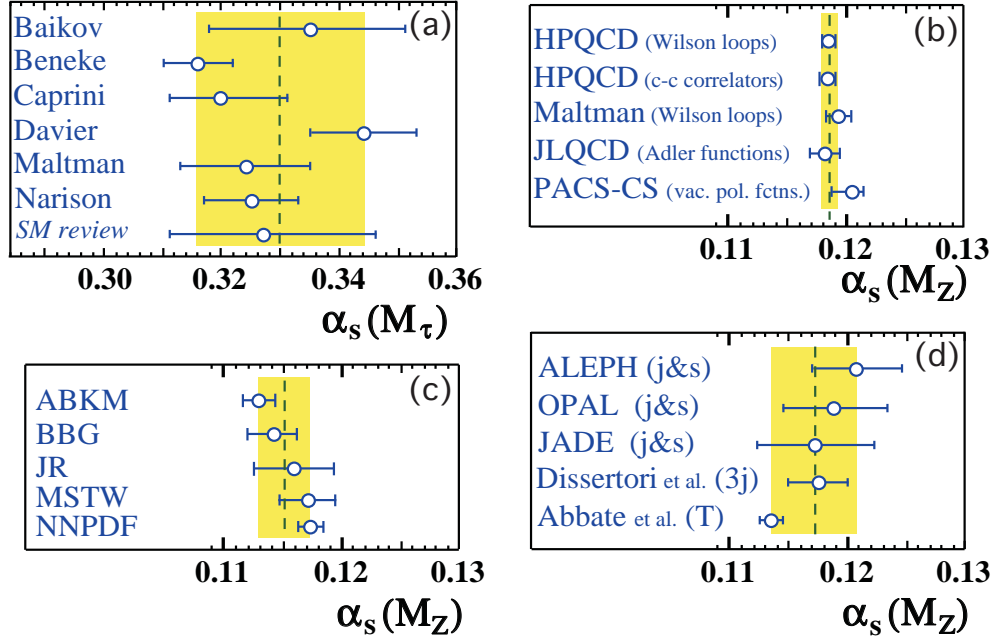
A summary of the  $e^+e^-$  results based on NNLO predictions is shown in Fig. 9.2(d). They average, according to the simple procedure defined above, to  $\alpha_s(M_Z^2) = 0.1172 \pm 0.0037$ .

#### *Hadron collider jets*

A determination of  $\alpha_s$  from the  $p_T$  dependence of the inclusive jet cross section in  $p\bar{p}$  collisions at  $\sqrt{s} = 1.96$  TeV, in the transverse momentum range of  $50 < p_T < 145$  GeV, based on NLO ( $\mathcal{O}(\alpha_s^3)$ ) QCD, led to  $\alpha_s(M_Z^2) = 0.1161^{+0.0041}_{-0.0048}$  [279], which is the most precise  $\alpha_s$  result obtained at a hadron collider. Experimental uncertainties from the jet energy calibration, the  $p_T$  resolution and the integrated luminosity dominate the overall error.

#### *Electroweak precision fits*

The N<sup>3</sup>LO calculation of the hadronic  $Z$  decay width was used in a revision of the global fit to electroweak precision data [280], resulting in  $\alpha_s(M_Z^2) = 0.1193 \pm 0.0028$ , claiming a negligible theoretical uncertainty. For this *Review* the value obtained in Sec. *Electroweak*



**Figure 9.2:** Summary of determinations of  $\alpha_s$  from hadronic  $\tau$ -decays (a), from lattice calculations (b), from DIS structure functions (c) and from event shapes and jet production in  $e^+e^-$ -annihilation (d). The shaded bands indicate the average values chosen to be included in the determination of the new world average of  $\alpha_s$ .

*model and constraints on new physics* from data at the  $Z$ -pole,  $\alpha_s(M_Z^2) = 0.1197 \pm 0.0028$  will be used instead, as it is based on a more constrained data set where QCD corrections directly enter through the hadronic decay width of the  $Z$ . We note that all these results from electroweak precision data, however, strongly depend on the strict validity of Standard Model predictions and the existence of the minimal Higgs mechanism to implement electroweak symmetry breaking. Any - even small - deviation of nature from this model could strongly influence this extraction of  $\alpha_s$ .

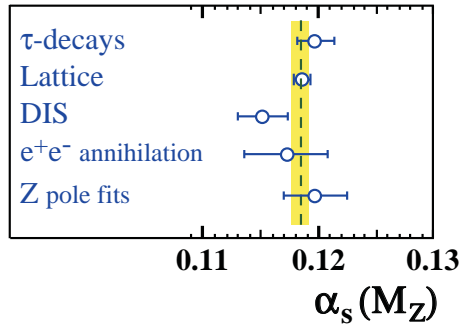
#### *Determination of the world average value of $\alpha_s(M_Z^2)$*

A non-trivial exercise consists in the evaluation of a world-average value for  $\alpha_s(M_Z^2)$ . A certain arbitrariness and subjective component is inevitable because of the choice of measurements to be included in the average, the treatment of (non-Gaussian) systematic uncertainties of mostly theoretical nature, as well as the treatment of correlations among the various inputs, of theoretical as well as experimental origin. In earlier reviews [243–245] an attempt was made to take account of such correlations, using methods as proposed, *e.g.*, in Ref. 281, and - likewise - to treat cases of apparent incompatibilities or possibly underestimated systematic uncertainties in a meaningful and well defined manner:

The central value is determined as the weighted average of the different input values. An initial error of the central value is determined treating the uncertainties of all individual measurements as being uncorrelated and being of Gaussian nature, and the

overall  $\chi^2$  to the central value is determined. If this initial  $\chi^2$  is larger than the number of degrees of freedom, i.e. larger than the number of individual inputs minus one, then all individual errors are enlarged by a common factor such that  $\chi^2/\text{d.o.f.}$  equals unity. If the initial value of  $\chi^2$  is smaller than the number of degrees of freedom, an overall, a-priori unknown correlation coefficient is introduced and determined by requiring that the total  $\chi^2/\text{d.o.f.}$  of the combination equals unity. In both cases, the resulting final overall uncertainty of the central value of  $\alpha_s$  is larger than the initial estimate of a Gaussian error.

This procedure is only meaningful if the individual measurements are known not to be correlated to large degrees, i.e. if they are not - for instance - based on the same input data, and if the input values are largely compatible with each other and with the resulting central value, within their assigned uncertainties. The list of selected individual measurements discussed above, however, violates both these requirements: there are several measurements based on (partly or fully) identical data sets, and there are results which apparently do not agree with others and/or with the resulting central value, within their assigned individual uncertainty. Examples for the first case are results from the hadronic width of the  $\tau$  lepton, from DIS processes and from jets and event shapes in  $e^+e^-$  final states. An example of the second case is the apparent disagreement between results from the  $\tau$  width and those from DIS [264] or from Thrust distributions in  $e^+e^-$  annihilation [278].



**Figure 9.3:** Summary of values of  $\alpha_s(M_Z^2)$  obtained for various sub-classes of measurements (see Fig. 9.2 (a) to (d)). The new world average value of  $\alpha_s(M_Z^2) = 0.1184 \pm 0.0007$  is indicated by the dashed line and the shaded band.

Due to these obstacles, we have chosen to determine pre-averages for each class of measurements, and then to combine those to the final world average value of  $\alpha_s(M_Z)$ , using the methods of error treatment as just described. The five pre-averages are summarized in Fig. 9.3; we recall that these are exclusively obtained from extractions which are based on (at least) full NNLO QCD predictions, and are published in peer-reviewed journals at the time of completing this *Review*. From these, we determine the new world average value of

$$\alpha_s(M_Z^2) = 0.1184 \pm 0.0007, \quad (9.23)$$

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with an uncertainty of well below 1 %<sup>\*\*\*</sup>. This world average value is - in spite of several new contributions to this determination - identical to and thus, in excellent agreement with the 2009 result [244]. For convenience, we also provide corresponding values for  $\Lambda_{\overline{MS}}$  suitable for use with Eq. (9.5):

$$\Lambda_{\overline{MS}}^{(5)} = (213 \pm 8) \text{ MeV} , \quad (9.24a)$$

$$\Lambda_{\overline{MS}}^{(4)} = (296 \pm 10) \text{ MeV} , \quad (9.24b)$$

$$\Lambda_{\overline{MS}}^{(3)} = (339 \pm 10) \text{ MeV} , \quad (9.24c)$$

for  $n_f = 5, 4$  and  $3$  quark flavors, respectively.

In order to further test and verify the sensitivity of the new average value of  $\alpha_s(M_Z^2)$  to the different pre-averages and classes of  $\alpha_s$  determinations, we give each of the averages obtained when leaving out one of the five input values:

$$\alpha_s(M_Z^2) = 0.1182 \pm 0.0007 \quad (\text{w/o } \tau \text{ results}), \quad (9.25a)$$

$$\alpha_s(M_Z^2) = 0.1183 \pm 0.0012 \quad (\text{w/o lattice results}), \quad (9.25b)$$

$$\alpha_s(M_Z^2) = 0.1187 \pm 0.0009 \quad (\text{w/o DIS results}), \quad (9.25c)$$

$$\alpha_s(M_Z^2) = 0.1185 \pm 0.0006 \quad (\text{w/o } e^+e^- \text{ results}), \text{ and} \quad (9.25d)$$

$$\alpha_s(M_Z^2) = 0.1184 \pm 0.0006 \quad (\text{w/o result from e.w. precision fit}). \quad (9.25e)$$

They are well within the error of the overall world average quoted above. Most notably, the result from lattice calculations, which has the smallest assigned error, agrees well with the exclusive average of the other results. However, it largely determines the size of the (small) overall uncertainty.

There are apparent systematic differences between the various structure function results, and also between the new result from Thrust in  $e^+e^-$  annihilation and the other determinations. Expressing this in terms of a  $\chi^2$  between a given measurement and the world average as obtained when *excluding* that particular measurement, the largest values are  $\chi^2 = 12.6$  and  $\chi^2 = 16.1$ , corresponding to 3.5 and 4.0 standard deviations, for the measurements of [265] and [278], respectively. We note that such and other differences between some of the measurements have been extensively discussed at a specific workshop on measurements of  $\alpha_s$ , however none of the explanations proposed so far have obtained enough of a consensus to definitely resolve the tensions between different extractions [282].

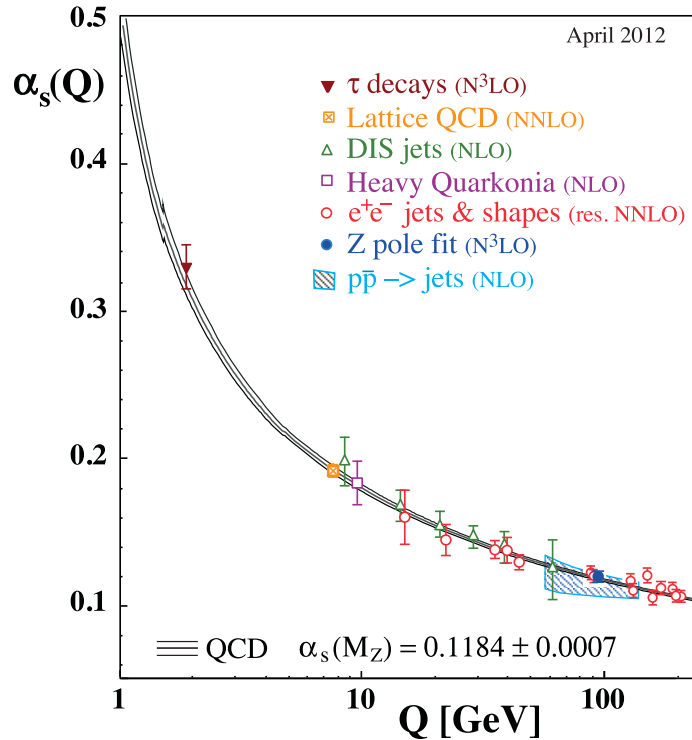
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<sup>\*\*\*</sup> The weighted average, treating all inputs as uncorrelated measurements with Gaussian errors, results in  $\alpha_s(M_Z^2) = 0.11844 \pm 0.00059$  with  $\chi^2/\text{d.o.f.} = 3.2/4$ . Requiring  $\chi^2/\text{d.o.f.}$  to reach unity leads to a common correlation factor of 0.19 which increases the overall error to 0.00072.

Notwithstanding these open issues, a rather stable and well defined world average value emerges from the compilation of current determinations of  $\alpha_s$ :

$$\alpha_s(M_Z^2) = 0.1184 \pm 0.0007 .$$

The results also provide a clear signature and proof of the energy dependence of  $\alpha_s$ , in full agreement with the QCD prediction of Asymptotic Freedom. This is demonstrated in Fig. 9.4, where results of  $\alpha_s(Q^2)$  obtained at discrete energy scales  $Q$ , now also including those based just on NLO QCD, are summarized and plotted.



**Figure 9.4:** Summary of measurements of  $\alpha_s$  as a function of the respective energy scale  $Q$ . The respective degree of QCD perturbation theory used in the extraction of  $\alpha_s$  is indicated in brackets (NLO: next-to-leading order; NNLO: next-to-next-to-leading order; res. NNLO: NNLO matched with resummed next-to-leading logs; N<sup>3</sup>LO: next-to-NNLO).

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