Scale Setting for $\alpha_s$ Beyond Leading Order

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Abstract

We present a general procedure for incorporating higher-order information into the scale-setting prescription of Brodsky, Lepage and Mackenzie. In particular, we show how to apply this prescription when the leading coefficient or coefficients in a series in the strong coupling $\alpha_s$ are anomalously small and the original prescription can give an unphysical scale. We give a general method for computing an optimum scale numerically, within dimensional regularization, and in cases when the coefficients of a series are known. We apply it to the heavy quark mass and energy renormalization in lattice NRQCD, and to a variety of known series. Among the latter, we find significant corrections to the scales for the ratio of $e^+e^-$ to hadrons over muons, the ratio of the quark pole to MS mass, the semi-leptonic $B$-meson decay width, and the top decay width. Scales for the latter two decay widths, expressed in terms of MS masses, increase by factors of five and thirteen, respectively, substantially reducing the size of radiative corrections.

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1 Introduction

QCD processes computed to a finite order in perturbation theory depend on both the choice of renormalization scheme and the scale for the running coupling constant $\alpha_s(q)$. In particular, changes in the scale induce variations at the first neglected order. While these variations diminish as higher orders are included, for low-order calculations they can be significant, particularly for processes sensitive to relatively low scales. Finding an optimum, physically motivated method for choosing this scale in such cases is important not only to produce accurate results, but also to reasonably estimate convergence based on the size of the series terms. Such a method allows a meaningful prediction or comparison with data even at leading order.

A variety of procedures have been proposed to select this scale [1]–[17]. In this paper, we investigate the prescription of Brodsky, Lepage and Mackenzie (BLM) [4]. In this method, one chooses the scale $q^*$ for $\alpha_s(q^*)$ which approximates the use of the fully dressed gluon propagator within that process. The choice is equivalent to determining the dominant momentum flowing through the propagator within a diagram [13, 16]. It has been applied successfully in a large variety of perturbative calculations. Among these, it was essential in demonstrating the viability of lattice perturbation theory [13], and in extracting a precise value of $\alpha_s$ from lattice simulations of the $\Upsilon$ and $\psi$ systems [18, 19].

In this paper, we generalize the prescription to remedy an anomaly observed in a variety of applications, particularly apparent when determining the scale over a range of parameters in the action. The NRQCD mass and energy renormalizations presented in Sect. 9.2 are typical examples. In most of these cases, for some value of the bare quark mass, the BLM scale diverges. We show that this breakdown is not a flaw in the general prescription, but rather the result of employing only a single vacuum-polarization insertion to estimate the typical momentum. While we focus on setting the scale for one-loop diagrams, we use information from two-loop and higher insertions within these diagrams to provide a simple generalization which accurately estimates the scale over the full range of parameters. It is straightforward to implement for both analytic and numerical computations, requiring only a modest extension beyond the leading order determination. For both computations, one obtains the additional information required from one higher moment in $\log(q^2)$ within the same diagram as was used in the lowest order application. For processes where the series coefficients are known, it requires only identifying the coefficient from vacuum polarization at the next order.

We note that other authors have developed a variety of extensions to Ref. [4], which explore conformal symmetry and the relation between various perturbative schemes [6, 10, 11], or which estimate nonperturbative contributions and resum classes of diagrams to all orders [13, 16]. Our goal is more modest: to provide a simple but robust scale determination for a process calculated to finite order. Specifically, we choose a single optimized scale for the leading, one-loop diagram, to be used for all orders. We show, however, that our prescription should effectively absorb into the leading term or terms the bulk of contribu-
tions from all higher order diagrams which dress the leading gluon.

2 General prescription

Following Refs. [4, 13], we choose the $V$ scheme based on the static-quark potential because of the direct connection between the scale of its coupling $\alpha_V$ and the momentum flowing through its associated gluon. For a one-loop diagram with an integrand $f(q)$ which contributes predominantly at large $q$, a natural choice for the scale $q^*$ of $\alpha_V$ is a mean value which reproduces the result of a fully dressed gluon within the diagram [4, 13],

$$\alpha_V(q^*) \int d^4q f(q) = \int d^4q \alpha_V(q) f(q),$$

as illustrated in Fig. 1. However, $\alpha_V(q)$ possesses a pole at $\Lambda_V$, an artifact of an all-orders summation of perturbative logarithms. We avoid this singularity by truncating the series for $\alpha_V(q)$ at a finite order, as is appropriate for an asymptotic series.

Expanding $\alpha_V(q)$ in terms of $\alpha_V(q^*)$

$$\alpha_V(q) = \frac{\alpha_V(q^*)}{1 + \alpha_V(q^*)\beta_0 \log(q^2/q^{*2})} \sim \alpha_V(q^*) - \alpha_V^2(q^*)\beta_0 \log(q^2/q^{*2}) + \cdots$$

and solving to first nontrivial order gives [13],

$$\log(q^{*2}) = \frac{\int d^4q f(q) \log(q^2)}{\int d^4q f(q)} \equiv \langle f(q) \log(q^2) \rangle \equiv \langle \log(q^2) \rangle,$$

a statement of this prescription suited for numerical calculations. Here

$$\beta_0 = \frac{1}{4\pi} \left( \frac{11}{3} C_A - \frac{4}{3} T_F n_f \right) = \frac{1}{4\pi} \left( 11 - \frac{2}{3} n_f \right),$$

and $\langle \rangle$ indicates an average weighted by $f(q)$.

By the definition of $\alpha_V$, Eq. (3) guarantees that $\alpha_V(q^*)$ absorbs the effect of second-order vacuum polarization insertions in the gluon’s propagator. An alternate method to determine $q^*$ is then to require that $\beta_0$, or equivalently $n_f$, disappears to that order [4]. This version is useful when the $\beta_0$ or $n_f$ dependence of coefficients in a perturbative expansion are known explicitly. We discuss this in more detail in Sect. 3.

Eq. (3) produces an optimum scale by means of an average of $\log(q^2)$ weighted by $f(q)$. As such, it provides a measure of the typical momentum carried by this gluon in the dominant integration region, in accord with intuition. However, in certain cases $\langle f \rangle$ vanishes, rendering $q^*$ from Eq. (3) meaningless. This is a consequence of using an expression first-order in $\alpha_V(q^*)$ for a process which is properly second-order, rather than a flaw in the general prescription. When $\langle f \rangle$ vanishes, the diagram on the left in Fig. 1 does not contribute. The leading
contribution from this gluon is second order, and the requirement that $q^*$ be chosen to best approximate the all-order result leads to the equation illustrated in Fig. 2. For an integrand dominated by large momentum, the left side of Eq. (1) is replaced by

$$-\alpha_\nu^2(q^*)\beta_0 \int d^4q f(q) \log(q^2/q^{*2}) ,$$

as is known from the running of $\alpha_\nu(q)$. Expanding $\alpha_\nu(q)$ as in Eq. (2) yields

$$\log(q^{*2}) = \langle f \log^2(q^2) \rangle + \alpha_\nu^2(q^*) \beta_0^2 \langle f \log(q^2) \rangle ,$$

This, rather than Eq. (3), is the appropriate statement of the prescription for this case.

As a simple illustration, consider a model in one dimension in which the Feynman diagram produces an integrand

$$f(q) = \delta(q - q_a) - \delta(q - q_b) ,$$

with positive $q_a$ and $q_b$. A reasonable expectation would be that $q^*$ should be some average of the contributing scales $q_a$ and $q_b$, particularly if they are nearby. Because $\langle f \rangle$ vanishes identically, Eq. (3) produces a divergent $q^*$, whereas Eq. (2), which begins with the next order contribution, gives for $q^*$ the more reasonable geometric mean

$$q^* = \sqrt{q_a q_b} .$$

This is the same scale obtained by Eq. (3) applied to the positive integrand

$$f(q) = \delta(q - q_a) + \delta(q - q_b) ,$$

as might be expected.

In other cases, while not strictly vanishing, $\langle f \rangle$ may be anomalously small, and the dominant contribution from this gluon is still as in Fig. 2. It is useful to generalize the lowest order prescription of Eq. (3) to incorporate both these cases naturally, and also to anticipate the situation where $\langle f \log(q^2) \rangle$ is anomalously small.

The discrepancy between the left and right sides of Eq. (1) relative to the lowest order term $\alpha_\nu(q^*) \int d^4q f(q)$ is

$$-\alpha_\nu^2(q^*)\beta_0 \langle \log(q^2/q^{*2}) \rangle + \alpha_\nu^2(q^*)\beta_0^2 \langle \log^2(q^2/q^{*2}) \rangle$$

Applying Eq. (3) leaves a leading difference of

$$\alpha_\nu^2(q^*)\beta_0^2 \langle [\log(q^2) - \langle \log(q^2) \rangle]^2 \rangle \equiv \alpha_\nu^2(q^*)\beta_0^2 \sigma^2$$

with $\sigma$ the standard deviation of $\log(q^2)$ with respect to the weight $f(q)/\langle f \rangle$. When $f(q)$ does not change sign, $f(q)/\langle f \rangle$ and $\sigma^2$ are both positive. When $f(q)$
changes sign and \( \langle f \rangle \) is anomalously small due to cancellations, this error can become arbitrarily large, indicating that treating this as a first order process is invalid and it is useful to incorporate information from the next order.

Matching the gluon’s contribution to next order to the fully dressed gluon, as in Fig. 3 adds the term in Eq. (10) to the left side of Eq. (1). Expanding both sides in terms of \( \alpha_V(q^*) \) as before leads to a leading relative difference of

\[
\alpha_V^2(q^*) \beta_0^2 \langle \log^2(q^2/q^{*2}) \rangle = -\alpha_V^2(q^*) \beta_0^2 \left[ \log^2(q^{*2}) - 2 \langle \log(q^2) \rangle \log(q^{*2}) + \langle \log^2(q^2) \rangle \right].
\]

When \( f(q)/\langle f \rangle \) is positive for all \( q \), this discrepancy is also strictly positive, and the best that can be done is to choose \( q^* \) to minimize it. The result of minimization is again just Eq. (11).

However, when \( f(q) \) possesses significant sign changes, the error in Eq. (12) can become negative for certain values of \( \log(q^{*2}) \), and minimization is not appropriate. In this case, it is possible to eliminate the difference altogether by
Choosing one of the two solutions

$$\log(q^2) = \left(\langle f \log(q^2) \rangle \pm \left(\langle f \log(q^2) \rangle - \langle f \rangle \langle f \log^2(q^2) \rangle\right)^{\frac{1}{2}}\right)^{\frac{1}{2}}$$

$$\equiv \langle \log(q^2) \rangle \pm \left(\langle \log(q^2) \rangle^2 - \langle \log^2(q^2) \rangle\right)^{\frac{1}{2}}$$

$$\equiv \langle \log(q^2) \rangle \pm [-\sigma^2]^{\frac{1}{2}}.$$  \hspace{1cm} (13)

When the logarithmic moments are available over a range of parameters, requiring that \( q^* \) be continuous and physically sensible makes the proper choice apparent, as will be observed below. In particular, when \( \langle f \rangle \) is nearly zero, this requires choosing the sign opposite to that of \( \langle \log(q^2) \rangle \). In every case we have considered, the choice has been obvious. However, if the need arises, one may resolve the sign unambiguously by using information from higher moments, as discussed in Sect. 7.

Were \( f(q) \) a probability distribution, \( \sigma \) would be its standard deviation. A negative value for \( \sigma^2 \) indicates that \( f(q)/\langle f \rangle \) has substantial changes of sign and is behaving significantly unlike a probability distribution. In this case, \( \langle f \rangle \) will be anomalously small, the order \( \alpha^2_s(q^*) \) contribution becomes important, and Eq. \( (13) \) provides the appropriate choice of scale. As a result, Eq. \( (13) \) determines \( q^* \) when \( \sigma^2 \) is negative, Eq. \( (3) \) when positive. This prescription is the main result of this paper.

Although Eq. \( (13) \) uses information from part of the next order, it is the appropriate scale to use when \( \sigma^2 \) is negative, even if only computing to first order in \( \alpha_s(q^*) \). In that case, in addition to setting the scale for the leading term, it allows for a reasonable estimate of the magnitude of the neglected next-order terms, based on \( \alpha^2_s(q^*) \). When \( \langle f \rangle \) is very small, these neglected terms should give a sizable correction to the first-order term. And when one computes to order \( \alpha^2_s(q^*) \) or higher using this scale, higher-order terms which dress the leading gluon should be small, having been largely absorbed into the first two, as in Fig. 3.
Figure 4: The BLM scale $q^*$ for the model of Eq. (14) as a function of $c$, with $q_a = 2.0$ and $q_b = 1.8$. The first order solution of Eq. (3) determines $q^*$ for $c < -1$, the second order solution of Eq. (13) for $c > -1$. The dark dotted lines show the first-order solution in regions in which it does not apply; light dotted lines display inapplicable second-order solutions.

As an illustration, we consider a slightly more general version of the model of Eq. (7),

$$f(q) = (1 + c)\delta(q - q_a) - \delta(q - q_b),$$  \hspace{1cm} (14)

where $\langle f \rangle$ vanishes exactly for $c = 0$, and has partial cancellation for $c > -1$. Figure 4 presents the scale $q^*$ determined by Eq. (3) when $\sigma^2 > 0$ and by Eq. (13) when $\sigma^2 < 0$; that is, when $c > -1$. For $c < -1$, with no cancellations, Eq. (3) produces reasonable values for $q^*$. It falls between $q_a$ and $q_b$, approaching $q_a$ for $|c|$ large, and $q_b$ for $c = -1$. As $c$ approaches zero and $\langle f \rangle$ vanishes, $q^*$ from this prescription diverges. However, for $c > -1$, $\sigma^2$ is negative, and Eq. (13) provides the optimum scale. It evidently behaves according to expectations. Even for the case when $c$ is large and positive and Eq. (3) produces a fairly sensible result, it overestimates $q^*$ and Eq. (13) is preferable.

To summarize, we restate the prescription in a more compact form. We have chosen inclusion of the running coupling within the integrand for a first-order diagram, $\int d^4q \, \alpha_V(q) \, f(q)$, as a natural means to account for the running of the coupling with the gluon’s momentum. It has the advantage that it incorporates higher-order diagrams which dress the gluon, has no arbitrary scale dependence, and appropriately accounts for the strength of the coupling of a gluon with momentum $q$.

It has the disadvantage that $\alpha_V(q)$ has an unphysical pole at $q = \Lambda_V$, making...
We avoid this by expanding $\alpha_V(q_*)$ at the scale $q_*$ as in Eq. (2), and working to finite order in $\alpha_V(q_*)$, giving

$$
\int d^4q f(q) \left[ \alpha_V(q_*) - \beta_0 \alpha^2_V(q_*) \log(q^2/q_*^2) + \beta_0^2 \alpha^3_V(q_*) \log^2(q^2/q_*^2) + \cdots \right].
$$

(15)

We choose $q_*$ to reproduce the full integral as well as possible. In the absence of significant cancellations in $\int d^4q f(q)$, we may select the scale by Eq. (3) so that the first non-leading term in Eq. (15) vanishes. The discrepancy is then the term of order $\alpha^3_V(q_*)$, which this choice for $q_*$ minimizes. Furthermore, as $q_*$ will be near the typical $q$, $f(q)$ will be roughly even about $q_*$, and higher-order contributions should be either near zero or their minimum depending on whether they are even or odd in $\alpha_V(q_*)$.

However, when $f(q)$ is essentially odd about some $q$ and so suffers from significant cancellations, this is not an appropriate prescription. The leading term in Eq. (15) will be anomalously small compared to the second term; in extreme cases, it might even vanish, and it would no longer make sense to absorb the second term into the leading term. Furthermore, the scale from Eq. (3) would no longer accurately represent the typical momentum, and neglected higher order terms in Eq. (15) would be anomalously large. It is, however, possible and sensible to require the third term to vanish by Eq. (6); that is, to absorb it into the second. This again provides a typical scale about which, in this case, $f(q)$ is essentially odd, minimizes the fourth-order term, and suppresses higher-order terms.

3 Schemes other than $V$

For prescriptions other than $\alpha_V$, vacuum polarization insertions will in general contribute subleading constants in addition to terms as in Eq. (5). Though nonleading, these constants can make significant contributions at physically interesting values of $q^2$, and so the optimum scale ought to be chosen to account for them as well. One method for doing so is to focus on the fermion loop [4]. Both the $\log(q^2)$ and the subleading constant will appear multiplied by $n_f$. Replacing $n_f$ with $\beta_0$ using Eq. (4) modifies the fermion loop contribution by a constant, to

$$
- \alpha_s(q^*) \beta_0 \left( \log(q^2/q_*^2) + a \right).
$$

(16)

When applying the first-order prescription, amending Eq. (3) to

$$
\log(q^2) = \langle \log(q^2) + a \rangle
$$

(17)

absorbs both the leading log and subleading constant into $\alpha_s(q^*)$. For $\overline{\text{MS}}$

$$
q_{\overline{\text{MS}}}^* = \exp(-5/6) q_V^* = 0.43 \ q_V^*.
$$

(18)

As with $\alpha_V$, this also absorbs the log associated with gluon vacuum polarization, since $\beta_0$ determines its contribution relative to the fermion loop. However,
the gluonic subleading constant need not contribute in this ratio, and so will not also be completely absorbed. One might choose instead to completely absorb the gluonic constant by solving Eq. (4) for the adjoint Casimir constant $C_A = N$ associated with the gluon loop in terms of $\beta_0$, before absorbing the $\beta_0$ term into $\alpha_s(q^*)$. This would be particularly appropriate when $n_f = 0$, for example. For $\overline{\text{MS}}$, the result is a factor of $\exp(-31/66) = 0.63$, not greatly different from Eq. (18). This indicates that to one loop, absorbing the fermion loop constant also largely accounts for the gluonic constant.

When applying the second-order prescription, a constant subleading contribution leads to the same shift in Eq. (13) as in Eq. (17), with

$$\log(q^2) = \langle\langle \log(q^2) + a\rangle\rangle \pm \left[\langle\langle \log(q^2)\rangle\rangle^2 - \langle\langle \log^2(q^2)\rangle\rangle\right]^{1/2}. \quad (19)$$

The second term on the right is invariant under a shift in $\log(q^2)$ by a constant, and so remains unaffected.

Because the $V$ scheme associates gluon exchange with a physical process at the specific scale $q^{*2}$, higher order contributions associated with the running of $\alpha_V$ must vanish identically when the gluon’s momentum hits $q^{*2}$. As a result, logarithmic contributions $\log(q^2/q^{*2})$ from these diagrams appear without subleading constants.

## 4 Determining $q^*$ in $\overline{\text{MS}}$

In order to provide a more realistic example, and to show how this prescription can be applied simply when using dimensional regularization, we determine $q^*$ for the one-loop $g\phi^3$ diagram of Fig. 5. While we use this as a simplified model for a quark self-energy diagram, we also note that this scale setting method is not restricted to QCD.

By introducing an additional denominator of the form $(q^2)^\delta$ into this diagram in $n$-dimensional Euclidean space,

$$\frac{g^2}{2} \int \frac{d^nq}{(2\pi)^n} \frac{1}{q^2 + m^2} \frac{1}{(p - q)^2 + m^2} \frac{1}{(q^2)^\delta}, \quad (20)$$
and expanding the result in \(\delta\) to second order, we produce the necessary logarithmic integrals:

\[
\langle f(q) \rangle - \delta \langle f(q) \log(q^2) \rangle + \frac{\delta^2}{2} \langle f(q) \log^2(q^2) \rangle + \ldots.
\]

(Note that Refs. [24, 14] present a different and elegant technique for extracting these logarithmic moments based on a simple dispersion sum over a fictional gluon mass.)

We evaluate Eq. (20) using standard methods and obtain

\[
\langle f(q) \rangle = -\frac{1}{\epsilon} + \int_0^1 dx \log\left(\frac{m^2 + x(1-x)p^2}{\mu^2}\right)
\]

\[
\langle f(q) \log(q^2) \rangle = \int_0^1 dx dy \left\{ -\frac{1}{\epsilon^2} + \frac{1}{\epsilon} \log\left(\frac{y}{\mu^2}\right) + \frac{\pi^2}{12} \right.
\]

\[
- \frac{1}{2} \log^2\left(\frac{y}{\mu^2}\right) + \frac{1}{2} \log^2\left(\frac{M^2}{y}\right) + \left[ 1 - \frac{x^2(1-y)^2p^2}{M^2} \right] \log\left(\frac{M^2}{y}\right)
\]

\[
\langle f(q) \log^2(q^2) \rangle = 2 \int_0^1 dx dy \left\{ -\frac{1}{\epsilon^3} + \frac{1}{\epsilon^2} \log\left(\frac{y}{\mu^2}\right) + \frac{\pi^2}{12} \right.
\]

\[
- \frac{1}{2} \log^2\left(\frac{y}{\mu^2}\right) + \frac{1}{6} \left[ -\psi''(1) - \frac{\pi^2}{2} \log\left(\frac{y}{\mu^2}\right) \right]
\]

\[
+ \log^3\left(\frac{y}{\mu^2}\right) + 3 \left[ 1 - \frac{x^2(1-y)^2p^2}{M^2} \right] \log^2\left(\frac{M^2}{y}\right) + \log^3\left(\frac{M^2}{y}\right) \right\}.
\]

In the above, we have dropped the overall factors \(g^2/(4\pi)^2\), which are here irrelevant, and substituted \(e^\gamma \mu^2/4\pi\) for \(\mu^2\). The latter greatly simplifies these expressions and allows us to apply the \(\overline{\text{MS}}\) prescription by subtracting the \(\epsilon\) poles alone, as one would for MS.

To renormalize these terms, we note that the \(\log(q^2)\) and \(\log^2(q^2)\) factors integrated within this one-loop diagram stand in for the large-momentum contributions of the first two higher-order vacuum polarization subdiagrams which
sum to form the running coupling. In particular, as these factors are finite, they represent these subdiagrams with their subdivergences already removed. For example, the factor $\log(q^2)$, which appears in the integrand which produced Eq. (23), comes from the large-momentum approximation to the $\overline{\text{MS}}$-renormalized one-loop vacuum polarization diagram; that is, to Eq. (24) without the pole. The poles in $\epsilon$ which remain in Eqs. (24) to (26) are then the new overall divergences associated with one, two and three loops, respectively. In the $\overline{\text{MS}}$ prescription these are simply discarded.

Finally, we note that Eq. (24) in this model is the one-loop vacuum polarization diagram in addition to being the particle’s self-energy. At large $p^2$, it is approximately $\log(p^2/\mu^2) - 2$, including the subleading constant. The constant $a$ in Eq. (17) is then $-2$, and the $\overline{\text{MS}}$ value for $q^*$ will differ by a factor $\exp(-1)$ from the expression for $q^*$ in the $V$ scheme.

While Eqs. (24) to (26) allow us to determine $q^*$ for any $p$ and $m$, it is illuminating to consider two limits. When $p^2 \gg m^2$, after renormalization and choosing $\mu^2 = p^2 \langle f(q) \rangle = -2$

$\langle \log(q^2) \rangle = \log(p^2) - \frac{\pi^2}{24}$

$\langle \log^2(q^2) \rangle = \log^2(p^2) - \pi^2 \log(p^2) + \left[ \frac{\psi''(1)}{6} - \frac{\pi^2}{12} + 2 \right]$

(27)

(28)

(29)

to leading order in $m^2/p^2$. These give

$$\sigma^2 = 2 + \frac{\psi''(1)}{6} - \frac{\pi^2}{12} \left[ 1 + \frac{\pi^2}{48} \right];$$

(30)

or numerically, $\sigma^2 = .6077$. The lowest order solution is then appropriate and yields a value for $q^*$ close to $p$, with

$$q^*/p = \exp(-1) \exp(-\pi^2/48) = .2995,$$

(31)

which corresponds to a value of $\exp(-\pi^2/48) = .8141$ in the $V$ scheme. We can use $\sigma$ to give a measure of the relative spread in the momenta which contribute to this diagram, with

$$\Delta q/q \approx \sigma/2 = .3898,$$

(32)

independent of the prescription. In general, when $p^2 \gg m^2$ but for $\mu^2$ arbitrary, $q^* \sim \sqrt{p \mu}$. This is the same result as Eq. (8), and reasonable for a diagram dominated by momenta between these two scales.

In the large mass limit $m \gg p$, with $\mu^2$ chosen to equal the natural scale $m^2$, we find

$$\langle f(q) \rangle = \frac{1}{6} \frac{p^2}{m^2}$$

(33)
\[ \langle f(q) \log(q^2) \rangle = \left( \frac{\pi^2 - 4}{4} \right) + \frac{1}{6} \log(m^2) \frac{p^2}{m^2} \]  

(34)

\[ \langle f(q) \log^2(q^2) \rangle = \left( \frac{\pi^2 - 4}{4} \right) \left[ 1 + \log(m^2) \right] - \frac{\psi''(1)}{3} \]  

(35)

\[ + \frac{1}{3} \left[ -1 + \frac{\pi^2}{6} + \frac{1}{2} \log^2(m^2) \right] \frac{p^2}{m^2} \]

to order \( p^2/m^2 \). Clearly in this limit \( \langle f(q) \rangle \) becomes anomalously small, and we expect the second order solution to be necessary. We confirm this by noting that to this order

\[ \langle f \rangle^2 \sigma^2 = -\left( \frac{\pi^2 - 4}{4} \right)^2 + \left[ \frac{\pi^2 - 4}{12} \right] - \frac{\psi''(1)}{18} \frac{p^2}{m^2} \]  

(36)

which is negative in this limit. The second order formula applies, and gives

\[ \log(q^*^2/m^2) = -2 + \left[ 1 - \frac{2\psi''(1)}{3(\pi^2 - 4)} \right] + \left[ \frac{\pi^2 - 3}{9(\pi^2 - 4)} \right] \]  

(37)

\[ + \frac{4\psi''(1)}{27(\pi^2 - 4)^3} (-3(\pi^2 - 4) + \psi''(1)) \frac{p^2}{m^2} \]

or numerically,

\[ q^*/m = 0.6953 + 0.0574 \frac{p^2}{m^2} \]  

(38)

For the \( V \) scheme, the leading \(-2\) in Eq. (37) is absent, and

\[ q^*_V/m = 1.8899 + 0.1562 \frac{p^2}{m^2} \]  

(39)

Fig. 6 and Fig. 7 display \( q^* \) as a function of \( p \) for the respective cases where \( \mu = p \) and \( \mu = m \). The limiting values discussed above are evident. For \( \mu = p \), the first-order solution determines \( q^* \) in both the large and small \( p \) regions, connected by the second-order solution in the interim. Immediately to the right of the point where the first-order solution diverges in Fig. 6, indicated by the vertical line, the second-order solution with positive root determines \( q^* \); to the left, the second-order negative root applies. For \( \mu = m \) (Fig. 7), the first-order solution applies for large \( p \), the negative root second-order solution for small \( p \). In both cases, use of the appropriate second order solution where applicable gives a meaningful and continuous value for \( q^* \) over the entire region in \( p \). Which second-order solution to choose from Eq. (13) is obvious.

Finally, we note that computing higher order average logs for this diagram requires only expanding Eq. (22) to higher orders in \( \delta \), without the need to compute additional diagrams.
Figure 6: The MS BLM scale $q^*/p$ as a function of momentum $p/m$ for the diagram of Fig. 5 in the scalar $\phi^3$ model, with $\mu = p$. The first-order solution determines $q^*$ in both the large and small $p$ regions, connected by the second-order solution in the interim. The vertical line indicates the point where the first-order solution diverges. The dark dotted lines show the first-order solution in the region in which it does not apply; light dotted lines display inapplicable second-order solutions.
Figure 7: The $\overline{\text{MS}}$ BLM scale $q^*/m$ as a function of momentum $p/m$ for the diagram of Fig. 5 in the scalar $\phi^3$ model, with $\mu = m$. The first-order solution determines $q^*$ in the large $p$ region, while the negative root second-order solution gives $q^*$ for small $p$. The dark dotted line shows the first-order solution in the region in which it does not apply; the light dotted line displays the inapplicable second-order solution.
5 Determining $q^*$ from a known series

To apply this prescription we need the first two logarithmic moments within the integrand associated with a gluon’s propagator. Under certain conditions, we may apply this prescription to set the scale for a process for which the expansion is already known by examining its $n_f$ dependence. At each order of $\alpha_V(\mu)$, the contribution from vacuum polarization will give the largest power of $n_f$, or equivalently, of $\beta_0$ \[4, 10\]. It is therefore possible to read off the logarithmic integrals directly from the series coefficients.

Using Eq. (4) to replace the largest-$n_f$ terms with $\beta_0$ in contributions associated with a particular gluon, we obtain a series of the form

$$c_0 \alpha_V(\mu) + (a_1 - c_1 \beta_0) \alpha_V^2(\mu) + (a_2 + \cdots + c_2 \beta_0^2) \alpha_V^3(\mu) + \cdots.$$ \tag{40}

The coefficients $c_n$ are then associated with vacuum insertions in the gluon propagator. Comparison with the right sides of Eqs. (1) and (2) gives

$$c_0 = \langle f \rangle,$$ \tag{41}
$$\frac{c_1}{c_0} \approx \langle \log(q^2/\mu^2) \rangle,$$ $$\frac{c_2}{c_0} \approx \langle \log^2(q^2/\mu^2) \rangle,$$

which holds when $f(q)$ contributes predominantly at large $q$. Given this association, the prescription to second order is

$$\log(q^2/\mu^2) = \frac{c_1}{c_0} \pm \left[ (\frac{c_1}{c_0})^2 - \frac{c_2}{c_0} \right]^{1/2}$$ \tag{42}

when the argument of the square root is positive, and

$$\log(q^2/\mu^2) = \frac{c_1}{c_0}$$ \tag{43}

otherwise.

For schemes other than $V$, the presence of a subleading constant $a$ contribution to fermion vacuum polarization leads to the identification

$$\frac{c_1}{c_0} \approx \langle \log(q^2/\mu^2) + a \rangle,$$ \tag{44}
$$\frac{c_2}{c_0} \approx \langle (\log(q^2/\mu^2) + a)^2 \rangle.$$

Because $c_1$ includes $a$ and the square root is insensitive to it, Eq. (43) and Eq. (44) automatically incorporate the shift in Eq. (4) and so may be used unchanged. Also, if one is able to identify in the series the constants $C_A$ associated with gluonic vacuum polarization, one could choose to use this instead to rewrite the series in terms of $\beta_0$. Eq. (43) and Eq. (42) would then automatically absorb the subleading gluonic constant, as discussed at the end of Sect. 4.

6 Combining series

Determining the scale for the series formed by multiplying two series,

$$F_a = 1 + c_a \alpha_V(q_a^*) + \cdots$$ \tag{45}
and
\[ F_b = 1 + c_b \alpha_v (q_b^*) + \cdots \] (46)
with known scales is straightforward when considering only first-order scale setting:
\[ F_{ab} \equiv F_a F_b = 1 + (c_a + c_b) \alpha_v (q_{ab}^*) + \cdots \] (47)
with
\[ \log(q_{ab}^*) = \frac{c_a \log(q_a^* q_{ab}^*) + c_b \log(q_b^* q_{ab}^*)}{c_a + c_b}. \] (48)

Because of the need to first test the sign of the new \( \sigma_{ab}^2 \), the prescription for applying second-order scale setting is slightly more involved. In that case,
\[ \sigma_{ab}^2 = c_a \langle \log^2(q^2) \rangle_a + c_b \langle \log^2(q^2) \rangle_b - \left( \frac{c_a \langle \log(q^2) \rangle_a + c_b \langle \log(q^2) \rangle_b}{c_a + c_b} \right)^2 \]
\[ = \frac{c_a \sigma_a^2 + c_b \sigma_b^2}{c_a + c_b} + \frac{c_a c_b}{(c_a + c_b)^2} \left( \langle \log(q^2) \rangle_a - \langle \log(q^2) \rangle_b \right)^2. \] (49)

As usual, if \( \sigma_{ab}^2 > 0 \), the first order combination
\[ \log(q_{ab}^*) = \frac{c_a \langle \log(q^2) \rangle_a + c_b \langle \log(q^2) \rangle_b}{c_a + c_b} \] (50)

applies. If \( \sigma_{ab}^2 < 0 \),
\[ \log(q_{ab}^*) = \frac{c_a \langle \log(q^2) \rangle_a + c_b \langle \log(q^2) \rangle_b}{c_a + c_b} \pm \left[ -\sigma_{ab}^2 \right]^\frac{1}{2}. \] (51)

When combining two series by division, \( F_{a/b} \equiv F_a / F_b \), the first-order coefficients subtract rather than add. The above formulas again apply, but with the replacement \( c_b \rightarrow -c_b \). These also apply to series combined by addition and subtraction, respectively, because the results at first order are equivalent.

For schemes other than \( V \), one should amend the average logs to include the subleading constants, as discussed in Sect. 3. The relation between the scale in \( V \) and in other schemes remains the same.

7 Higher orders

Extending this prescription beyond second order is relatively straightforward, though it requires computation of \( \langle \log^3(q^2) \rangle \) and higher moments, or information from third-order and higher terms in a known series. An extension to third order, for example, would be necessary should both \( \langle f \rangle \) and \( \langle f \log(q^2) \rangle \) vanish, making the third term in Eq. (13) the leading term. Absorbing the subsequent term by requiring \( \langle f \log^3(q^2/q^2) \rangle \) to vanish would give
\[ \log(q^2) = \frac{\langle f \log^3(q^2) \rangle}{3 \langle f \log^2(q^2) \rangle}, \] (52)
as one would also obtain from Fig. 3 with two loops on the left side.

When $\langle f \rangle$ and $\langle f \log(q^2) \rangle$ are not identically zero but are anomalously small relative to higher moments, requiring $\langle f \log^3(q^2/q^*^2) \rangle$ to vanish still gives the appropriate scale. A symptom that this is the case would be a third-order scale near Eq. (52) which shifts significantly the scale obtained at lower order, and which is more in line with physical expectations. If available, higher even moments near their minima or odd moments near zero at this scale would confirm it.

An order-$n$ equation is necessary to set $q^*$ only when all of the first $(n-2)$ moments vanish or are anomalously small. It would be unusual for a generic integrand $f(q)$ to be effectively orthogonal to more than a few powers of $\log(q^2)$, and so the need to use a high-order equation should be rare. We have found no realistic cases for which either Eqs. (3) or (13) were not sufficient.

In Fig. 8 we illustrate the appropriate scales for a model,

$$f(q) = A\delta(q - q_a) + B\delta(q - q_b) + (D + c)\delta(q - q_d),$$

(53)

with

$$B = -A\log(q_a/q_d)/\log(q_b/q_d), \quad D = -(A + B),$$

(54)

corrived such that both $\langle f \rangle$ and $\langle f \log(q^2) \rangle$ vanish at $c = 0$. The second- and third-order solutions behave as expected where appropriate; the first-order solution, while not divergent, is low throughout. The unphysical behavior of the first-order solution, as well as the significant discrepancy between first- and third-order scales indicate that the first-order result is inadequate.

Note the one- and two-node structures of the integrand $f(q)$ in the two- and three-delta models of Eq. (14) and Eq. (53), similar to generic first and second excited-state wavefunctions. This is the result of choosing $f(q)$ to be orthogonal to the zeroth, and to both the zeroth and first powers of $\log(q^2)$, respectively. Integrand requiring higher-order equations would necessarily have more nodes and additional detailed structure.

In general, higher-order solutions can confirm that a scale determined at a lower order is indeed typical. For example, in Fig. 4 we include the third order solution for the Eq. (14) model; where applicable, it does not differ significantly from the first-order result. This will also be apparent when we examine higher moments for certain processes in Sect. 9.

Thus far, for simplicity, we have restricted our discussion to contributions to $\alpha_V(q)$ from one loop vacuum polarization. We show here that the above expressions for $q^*$ are not limited to these. Specifically, including subleading contributions to $\alpha_V(q)$ expanded within a diagram as in Eq. (14) gives

$$\alpha_V(q^*) \langle f \rangle + \alpha_V^2(q^*) [\beta_0 \Delta_1] + \alpha_V^3(q^*) [\beta_0^2 \Delta_2 + \beta_1 \Delta_1]$$

$$+ \alpha_V^4(q^*) [\beta_0^3 \Delta_3 + \frac{5}{2} \beta_0 \beta_1 \Delta_2 + \beta_2 \Delta_1]$$

$$+ \alpha_V^5(q^*) [\beta_0^4 \Delta_4 + \frac{13}{3} \beta_0^2 \beta_1 \Delta_3 + 3 \beta_0 \beta_2 \Delta_2 + \frac{3}{2} \beta_1^2 \Delta_2 + \beta_3 \Delta_1] + \cdots.$$
Figure 8: The BLM scale $q^*$ for the model of Eq. (53) as a function of $c$, with $q_a = 2.0$, $q_b = 1.8$ and $q_d = 1.6$. The second-order solution determines $q^*$ for $c < -1$, the third-order solution for $c > -1$. The dark dotted line shows the first-order solution; light dotted lines display inapplicable second and third-order solutions.
Figure 9: The BLM scale for the δ-function model of Eq. (14) as in Fig. 4, but with the inclusion of the third-order solution. It is applicable for \( c < -1 \) and indicated by the additional dark line. Dotted lines indicate inapplicable solutions.

Here

\[
\beta_1 \equiv \frac{1}{(4\pi)^2} \left( 102 - \frac{38}{3} n_f \right),
\]

and

\[
\beta_2 \equiv \frac{1}{(4\pi)^3} \left( \frac{2857}{2} - \frac{5033}{18} n_f + \frac{325}{58} n_f^2 \right),
\]

and we have defined the moments

\[
\Delta_n \equiv \langle f \log^n(q^*/q^2) \rangle = \left( f \left[ \log(q^*) - \log(q^2) \right] \right)^n.
\]
should do reasonably well at approximating the right side of Eq. (1) regardless of the number of loops kept in the $\beta$ function for $\alpha V(q)$. When $\langle f \rangle$ vanishes or is anomalously small, it is inappropriate to absorb the leading correction at each logarithmic order into the vanishing or small first term. In this case Eq. (13) gives the appropriate scale. It causes $\Delta_2$ to vanish, and so absorbs the second correction at each logarithmic order into the set of leading corrections. Again, because Eq. (13) produces a typical scale, higher-order terms should be small.

This illustrates one of the advantages of using a coupling based on a physical process, such as $\alpha V$. For other schemes, there can be significant subleading constants associated with the diagrams which dress the gluon, not accounted for in the running coupling. These will appear, for example, in the coefficients associated with the leading log term at each order $n$; that is, with $\beta_0^{n-1}$, as

$$\Delta_n \equiv \langle f \left[ \log(q^*^2) - (\log(q^2) + a_0) \right]^n \rangle,$$

and one may absorb them by adjusting the scale. However, only one such constant can be absorbed in this manner; parts of those associated with $\beta_1$ and higher will remain. By its definition, these constants cannot appear for $\alpha V$, and $\alpha V(q^*)$ well represents the strength of a physical gluon at the scale $q^*$. This optimum choice of scale minimizes all coefficients associated with dressing the gluon, not just those associated with $\beta_1$.

8 Improving convergence

Thus far we have been considering the appropriate scale $q^*$ for the leading $\alpha V$. For the sake of simplicity, we will be content to optimize the scale for the leading term, and will use the same scale for higher-order diagrams. From the previous discussion, it is clear that this will be a reasonable scale for diagrams which dress the leading-order gluon; these contributions should be small, having been largely absorbed into the leading term or terms. There is no reason to believe, however, that it will be the best scale for other higher-order diagrams, and it should certainly be possible to improve the convergence of the series by choosing the scale for such diagrams separately [4, 10].

There are other cases for which it could prove advantageous to allow different scales at different orders, for different diagrams within the same order, or even within a single diagram. Returning to the simple and unexceptional model of Eq. (3), for which the first-order scale setting Eq. (3) gives Eq. (8), we note that the moments

$$\langle \log^n(q^*^2/q^2) \rangle = \frac{1}{2} \left[ \log^n(q^*^2/q_a^2) + \log^n(q^*^2/q_b^2) \right]$$

become zero for $n$ odd, and $\log^n(q_a/q_b)$ for $n$ even. The latter grow in magnitude when the $q_a$ is a few times greater than $q_b$. As these are proportional to the coefficients of terms which dress the gluon, terms in the series become $\approx 1$ when this range $q_a/q_b$ exceeds a few over $\alpha_s$. The series becomes badly behaved then
not only when the scale for $\alpha_s$ is low, but also when the range of important momenta is large [14, 16].

Nevertheless, in this simple case the remedy is obvious. The problem results from requiring $\alpha_s$ at a single scale to incorporate two widely different scales. Separating these and writing the series for this model in terms of both $\alpha_s(q_a)$ and $\alpha_s(q_b)$ incorporates vacuum polarization contributions exactly and causes higher moments to vanish. This reinforces the idea that for a series in which gluons from different diagrams occur in loops sensitive to significantly different momenta, allowing the $\alpha_s$ associated with each to have its own scale could improve the series’ convergence. Furthermore, for a series in which a gluon in a single diagram is sensitive to a wide range of momenta one might even consider improving its behavior by splitting up the integrand, with $\alpha_s$ at a different scale assigned to each region, as in the example above.

Even for diagrams which dress a specific gluon, it is possible to minimize higher moments by allowing the scale associated with these diagrams to differ at different orders. In particular, one may select the scale at every other order such that the following moment vanishes, and the next is minimized. Variations in the scale would account for the different regions the moments probe in the integrand.

We will not pursue this further here, but mention that care must be taken to preserve gauge invariance if separate scales are assigned to different parts of a series.

9 Applications

9.1 Known series

In Table 9 we present a collection of results for perturbative quantities for which at least the second logarithmic moment is available, allowing us to apply scale setting beyond lowest order. Ref. [10] presents a useful compilation and discussion of many of these. These include the log of the $1 \times 1$ Wilson loop in lattice QCD ($-\log W_{11}$) [13, 22], the ratio of $e^+ e^-$ goes to hadrons over muons $(R_{e^+ e^-})$ [20, 21], the ratio of the quark pole mass to its $\overline{MS}$ mass $(M/M)$ [31, 37] and [16], the ratio of $\tau$ goes to $\nu_\tau +$ hadrons over $\tau$ goes to $\nu_\tau e^- \nu_\tau (R_\tau)$ [37–39, 12, and 29, 30, 15], the semileptonic $B$-meson decay width $(\Gamma (B \rightarrow X_u \nu))$ [43, 44, 6] expressed both in terms of the pole and $\overline{MS}$ $b$-quark masses, the top quark decay width $(\Gamma (t \rightarrow bW))$ [51–56 and 24, 46, 14] in terms of its pole and $\overline{MS}$ masses, the Bjorken sum rules for polarized electroproduction $(\int_0^1 dx [g_1^{p}(x,Q^2) - g_1^{n}(x,Q^2)])$ [57–59, 22], and deeply inelastic neutrino-nucleon scattering $(\int_0^1 dx [F_1^p(x,Q^2) - F_1^n(x,Q^2)])$ [60, 61, 62], and the static quark potential $(V(Q^2))$ [25, 28 and 57, 68].

We note that the non-singlet part of the Ellis-Jaffe sum rule [69–72] and [62] gives the same scale as the former Bjorken sum rule, the Gross-Llewellyn Smith sum rule [73–75, 12] the same scale as the latter.

All but the first scales are from known $\overline{MS}$ series, and for these at least
the fermion vacuum polarization graphs must be given to two loops. In several cases higher logarithmic moments are known, which will allow us to test the consistency of the procedure. We find four cases where the second-order formula gives the preferred scale.

When the first-order solution is appropriate, the second moment gives a rough measure of the range in momenta which flow through the gluon, with

$$\frac{\Delta q}{q} \approx \frac{1}{2} \left( \frac{\Delta_2}{\langle f \rangle} \right)^{\frac{1}{2}}. \quad (61)$$

Here, $\Delta q$ is the standard deviation in $q$ and $\Delta_2$ is defined in Eq. (58). A large range results in large coefficients at higher orders, as discussed above. When the second-order scale is appropriate, Eq. (61) clearly is not. However, if higher moments are available, we may estimate this range using

$$\frac{\Delta q}{q} \approx \left| \frac{\Delta_{n+2}}{4(n+1)\Delta_n} \right|^{\frac{1}{2}}, \quad (62)$$

with $n$ odd. In Table 1, we use $n = 1$. This expression gives the standard deviation in a distribution modelled by a Gaussian times $[\log(q^2) - \log(q^2)]^n$ to render it odd. We found it to give reasonably consistent results for various $n$ when applied to several examples discussed below, though other measures are certainly possible.

For $R_{\tau - \mu}$, $M/\bar{M}$, and both $\Gamma(B \rightarrow X_u e\bar{\nu}_e)$ and $\Gamma(t \rightarrow bW)$ expressed in terms of MS masses, we find that the second-order scale is appropriate, leading to significant corrections to the anomalously low first-order scales, especially in the latter three. While the new scale for $M/\bar{M}$ is significantly increased, we note that $\Delta q/q$ is still relatively large, indicating sensitivity to low-momentum scales even when $M$ is large, and threatening a poorly behaved series. This apparently infects the $b$ and $t$ decay rates when expressed in terms of pole masses, as shown by their low scales. By contrast, MS masses behave more as bare masses, being sensitive to short distances; expressing the two decays in terms of these significantly improves their behavior [55, 74, 24, 14, 15]. This is clear from both their scales and widths. Both these series should be well-behaved, and well-represented by $\alpha_s$ at a single, physically reasonable scale. But it is necessary to use second-order scale setting to see this; the first-order $q^*$ for each indicates a scale which is misleadingly low.

Refs. [14, 13, 17] provide very useful values for fermion vacuum polarization contributions, and therefore logarithmic moments, computed to eighth order for the pole to MS ratio, $\tau$, $B$ and $t$ decays. These allow us to compute their $\Delta q$’s using Eq. (62), but more importantly, to confirm the general picture as discussed in Sect. 3. In Fig. 10 we use this information to display the first eight moments $[\log(q^2) - \log(q^2)]^n$ as functions of $\log(q^2/M^2_b)$ for $\Gamma(B \rightarrow X_u e\bar{\nu}_e)$ expressed in terms of the MS mass $\bar{M}_b$. Here $q^2_b$ absorbs the fermion loop constant associated with the MS prescription, as in Eq. (18), and $M_b$ is the $b$-quark pole mass. We observe that choosing $\log(q^2_b/M^2_b)$ to set the second moment to zero
using Eq. (13) not only removes it and minimizes the third moment, it also sets all of the higher moments near their minima or zeros. It is clear that this is the natural scale for this process, and that terms beyond second order which dress the leading gluon should be small. The first moment is clearly anomalous, and setting it to zero using Eq. (9) would evidently lead to large higher-order corrections. In general, we expect $f(q)$ to be either roughly even or odd about its typical scale $q^*$, and the sign of the second moment, $\sigma^2$, should distinguish the two. For $\Delta q$ sufficiently small, using Eq. (3) or Eq. (13) depending on the sign of $\sigma^2$ should give reasonable values except in very rare cases.

The picture for $M/\bar{M}$, Fig. 11, is similar. While choosing the second order scale is more appropriate than first, causing the second moment to vanish and minimizing the third, the zeros and minima of higher moments drift progressively lower. Such behavior is anticipated by the relatively large value of $\Delta q/q$, which indicates a wide range of contributing momenta. In this case, higher moments are increasingly sensitive to lower $q$, and the corresponding coefficients will progressively increase. We might improve the convergence of the series by methods discussed in Sect. 8. For example, choosing $q^*$ separately at each odd order in $\alpha_s$, causing the following even moment to vanish and minimizing the subsequent odd moment, with each $q^*$ indicating the characteristic scale for that moment. An alternative is to resum the entire set of polarization diagrams [14, 16]. Regardless, the ability to detect sensitivity to a large range of momenta, in addition to the scale itself, by computing the first few logarithmic moments is sufficient to warn of large higher order corrections. In this case, it suggests using $\bar{M}$ rather than $M$ in expressions for $b$ and $t$ decays.

9.2 Quark mass and energy renormalization in lattice NRQCD

Lattice Nonrelativistic QCD (NRQCD) is an effective field theory designed to reproduce the results of continuum QCD for a heavy quark at energies small relative to its mass [75, 76, 77]. Higher-dimensional operators provide systematic corrections ordered by quark velocity $v$ and lattice spacing $a$, and account for radiative processes above the cutoff, typically around the mass. For a cutoff much larger than $\Lambda_{QCD}$, lattice perturbation theory should give reliable values for the coefficients of these operators as well as the renormalization factors which connect bare to physical quantities. Ref. [13] demonstrates that this expectation is valid, provided one uses a renormalized rather than bare coupling constant, and divides link gauge fields by their mean value to remove large tadpole contributions peculiar to the lattice.

Refs. [78] to [80] present calculations of two of these quantities to first order in $\alpha_s$: the renormalization factor $Z_m$, which connects the bare lattice heavy quark mass to its pole mass, and $E_0$, the shift from zero of the nonrelativistic energy of a heavy quark at rest. Ref. [80], using an action improved to $O(v^2)$ and $O(a^2)$, and to $O(v^4)$ for spin-dependent interactions, found that first-order scale setting produced anomalous results for certain values of the bare mass, particularly after tadpole improvement.

In Tables 2 to 5 and Figures 12 to 15, we present new values for the scale for
Table 1: Applications of second-order scale setting to several processes. The coefficients $c_n$ are defined in Sect. 5. $q^*_1$ gives the scale set by Eq. (3). $q^*_2$ gives the preferred scale by Eq. (13) where appropriate, also indicated by boxes. $\Delta q$ measures the range of momentum running through the gluon.

|                | $c_1/c_0$ | $q^*_1$ | $c_2/c_0$ | $\sigma^2$ | $q^*_2$ | $\Delta q$ |
|----------------|-----------|--------|-----------|-----------|--------|----------|
| $-\log W_{11}$ | 2.448     | 3.402/a| 6.316     | 0.3194    | –      | 0.96/a   |
| $R_{e+e-}(s)$  |           |        |           |           |        |          |
| $-0.69172$     | 0.7076$\sqrt{s}$ | $-0.186421$ | $-0.66497$ | 1.064$\sqrt{s}$ | –      |
| $M/M$          |           |        |           |           |        |          |
| $-4.6862$      | 0.09603M | 17.623 | $-4.3374$ | $0.27205M$ | 0.38M  |
| $R_{\tau}$     |           |        |           |           |        |          |
| $-2.2751$      | 0.32060M$\tau$ | 5.6848 | 0.50872   | –         | 0.11M$\tau$|
| $\Gamma(B \rightarrow X_a e\bar{\tau})/M_b^5$ | $-5.3382$ | 0.06932M$b$ | 34.410 | 5.9139 | – | 0.084M$b$ |
| $\Gamma(B \rightarrow X_a e\bar{\tau})/M_b^5$ | $-4.3163$ | 0.11554M$b$ | 8.0992 | $-10.531$ | $0.58534M_b$ | 0.35M$b$ |
| $\Gamma(t \rightarrow bW)/M_t^3$ | $-4.2054$ | 0.12213M$t$ | 23.046 | 5.3611 | – | 0.14M$t$ |
| $\Gamma(t \rightarrow bW)/M_t^3$ | $-5.7076$ | 0.05763M$t$ | 6.0996 | $-26.477$ | $0.75502M_t$ | 0.34M$t$ |
| $\int_0^1 dx [g_1^{cp}(x, Q^2) - g_1^{en}(x, Q^2)]$ | $-2$ | $e^{-1}Q = 0.3679Q$ | 115/18 | 43/18 | – | 0.28Q |
| $\int_0^1 dx [F_1^{cp}(x, Q^2) - F_1^{en}(x, Q^2)]$ | $-8/3$ | $e^{-4/3}Q = 0.2636Q$ | 155/18 | 3/2 | – | 0.16Q |
| $V(Q^2)$       | $-5/3$   | $e^{-5/6}Q = 0.4346Q$ | 25/9 | 0 | – | 0 |
Figure 10: The moments $\left|\left\langle \left[\log(q^2_{\text{MS}}) - \log(q^2)\right]^n\right\rangle\right|^{1/n}$ as functions of $\log(q^2_{\text{MS}}/M^2_b)$ for $n = 1$ to 8 (left to right) for $\Gamma(B \to X_u e\nu_e)$ over the $\overline{\text{MS}}$ mass $M_b$. The vertical line indicates the choice for the scale $\log(q^2_{\text{MS}}/M^2_b)$ using Eq. (13). By choosing the second-order prescription such that the second moment vanishes, $\log(q^2_{\text{MS}}/M^2_b)$ is either near the minimum or the zero for all higher moments, minimizing higher-order terms in Eq. (13).
Figure 11: The moments $\langle \langle \log(q^2_{\text{MS}}) - \log(q^2) \rangle^n \rangle^{1/n}$ as functions of $\log(q^2_{\text{MS}}/M^2)$ for $n = 1$ to 8 (left to right) for $M/M$. The vertical line indicates the choice for the scale $\log(q^2_{\text{MS}}/M^2)$ using Eq. (13).
a variety of bare quark masses $M_0$, both with and without tadpole improvement. By applying Eq. (13) in regions where appropriate, we obtain a reasonable scale for all values of $M_0$, correcting the anomalies observed in Ref. [80]. As expected, there is a significant reduction in the scale after tadpole improvement. The tadpole contributions to these renormalizations are quadratically divergent in the inverse lattice spacing, and so are generally large and sensitive to large momenta. Tadpole improvement is designed to remove the bulk of these contributions, and so reduces the typical scale from 2 – 4 to 0.5 – 1.5 in units of the inverse lattice spacing $a$.

10 Conclusions

In this paper we have derived a method which incorporates information from higher orders into the general prescription of Ref. [4] for choosing the optimal scale $q^*$ for the strong coupling constant $\alpha_s$. We find that it corrects erroneous scales where the leading term or terms are anomalously small.

The extended prescription states that Eq. (13) determines the optimal scale $q^*$ when the argument of the square root is positive. When it is not, the first
Figure 13: The BLM scale $q^*$ for the pole mass renormalization factor $Z_m$ as a function of the bare lattice mass $aM_0$ in NRQCD with tadpole improvement. The first order solution determines $q^*$ between $aM_0 = 2.00$ and 3.50, the second order elsewhere. Circles indicate the appropriate scale; triangles indicate the first-order solution in regions where it does not apply.
Figure 14: The BLM scale $q^*$ for the energy shift $E_0$ as a function of bare lattice mass $aM_0$ in NRQCD without tadpole improvement. The first order solution determines $q^*$ for all values.
Figure 15: The BLM scale $q^*$ for the energy shift $E_0$ as a function of bare lattice of the bare lattice mass $aM_0$ in NRQCD with tadpole improvement. The first order solution determines $q^*$ between $aM_0 = 0.80$ and 1.70, the second order elsewhere. Circles indicate the appropriate scale; triangles indicate the first-order solution in regions where it does not apply.
Table 2: The BLM scale for the pole mass renormalization factor $Z_m$ for several values of the bare lattice mass $aM_0$ in NRQCD without tadpole improvement. $aq_1^*$ gives the scale set by Eq. (3) in units of the inverse lattice spacing. $aq_2^*$ gives the preferred scale by Eq. (13) where appropriate. The parameter $n$ is set to ensure the stability of heavy quark propagator evolution in simulations [76].

| $n$ | $aM_0$ | $(f) \equiv (Z_m - 1)/\alpha_s$ | $\langle f \log((aq)^2) \rangle$ | $\langle f \log^2((aq)^2) \rangle$ | $aq_1^*$ | $aq_2^*$ |
|-----|--------|----------------------------------|---------------------------------|---------------------------------|--------|--------|
| 1   | 20.00  | 0.4679(39)                       | 1.343(11)                       | 4.091(62)                       | 4.202(71) | -      |
|     | 17.50  | 0.4860(34)                       | 1.364(10)                       | 4.196(65)                       | 4.068(58) | -      |
|     | 15.00  | 0.5125(30)                       | 1.3907(85)                      | 4.211(41)                       | 3.883(44) | -      |
|     | 12.50  | 0.5410(46)                       | 1.426(14)                       | 4.242(63)                       | 3.736(65) | -      |
|     | 10.00  | 0.5880(35)                       | 1.463(12)                       | 4.384(68)                       | 3.469(43) | -      |
|     | 7.00   | 0.7057(17)                       | 1.5423(58)                      | 4.880(32)                       | 2.982(15) | -      |
|     | 5.00   | 0.8624(14)                       | 1.7153(48)                      | 5.538(29)                       | 2.7034(87) | -    |
|     | 4.00   | 1.0071(27)                       | 1.9021(70)                      | 6.062(32)                       | 2.571(11) | -      |
| 2   | 4.00   | 1.0177(23)                       | 1.9264(80)                      | 6.164(33)                       | 2.577(11) | -      |
|     | 3.50   | 1.1268(23)                       | 2.0710(83)                      | 6.614(53)                       | 2.507(10) | -      |
|     | 3.00   | 1.2853(21)                       | 2.2859(68)                      | 7.351(35)                       | 2.4333(74) | -    |
|     | 2.70   | 1.4119(19)                       | 2.4540(79)                      | 7.911(34)                       | 2.3846(73) | -    |
|     | 2.50   | 1.5188(23)                       | 2.6141(74)                      | 8.390(52)                       | 2.3646(66) | -    |
|     | 2.00   | 1.9018(22)                       | 3.1745(79)                      | 10.214(32)                      | 2.3039(53) | -    |
|     | 1.70   | 2.2751(24)                       | 3.7546(75)                      | 12.039(56)                      | 2.2823(43) | -    |
|     | 1.60   | 2.4384(24)                       | 4.0086(79)                      | 12.857(39)                      | 2.2750(41) | -    |
|     | 1.50   | 2.6320(22)                       | 4.3141(78)                      | 13.745(37)                      | 2.2694(37) | -    |
| 3   | 1.40   | 2.8804(23)                       | 4.7587(76)                      | 15.073(37)                      | 2.2842(34) | -    |
|     | 1.20   | 3.5010(22)                       | 5.7986(83)                      | 18.143(39)                      | 2.2891(30) | -    |
|     | 1.00   | 4.4915(19)                       | 7.4780(68)                      | 23.109(31)                      | 2.2990(19) | -    |
| 5   | 0.80   | 6.3033(34)                       | 10.720(11)                      | 32.131(63)                      | 2.3405(24) | -    |
Table 3: The BLM scale for the pole mass renormalization factor $Z_m$ for several values of the bare lattice mass $aM_0$ in NRQCD with tadpole improvement. $aq^*_1$ gives the scale set by Eq. (3) in units of the inverse lattice spacing. $aq^*_2$ gives the preferred scale by Eq. (13) where appropriate. The parameter $n$ is set to ensure the stability of heavy quark propagator evolution in simulations [76].

| $n$ | $aM_0$ | $(f) \equiv (Z_m - 1)/\alpha_s$ | $\langle f \log((aq)^2) \rangle$ | $\langle f \log^2((aq)^2) \rangle$ | $aq^*_1$ | $aq^*_2$ |
|-----|--------|----------------------------------|---------------------------------|---------------------------------|--------|--------|
| 1   | 20.00  | -0.2381(39)                      | -0.385(11)                      | -0.367(62)                      | 2.246(61) | 1.34(11) |
|     | 17.50  | -0.2224(34)                      | -0.371(10)                      | -0.278(65)                      | 2.301(60) | 1.24(91) |
|     | 15.00  | -0.1996(30)                      | -0.353(85)                      | -0.286(41)                      | 2.422(61) | 1.26(73) |
|     | 12.50  | -0.1773(46)                      | -0.333(14)                      | -0.293(63)                      | 2.56(12)  | 1.29(13) |
|     | 10.00  | -0.1416(35)                      | -0.323(12)                      | -0.223(68)                      | 3.14(16)  | 1.21(12) |
|     | 7.00   | -0.0566(17)                      | -0.324(58)                      | 0.066(32)                       | 17.6(1.7) | 0.95(13) |
|     | 5.00   | 0.0386(14)                       | -0.3018(48)                     | 0.335(29)                       | 0.0201(31)| 0.75(17) |
|     | 4.00   | 0.1126(27)                       | -0.2881(70)                     | 0.413(32)                       | 0.278(12) | 0.65(50) |
| 2   | 4.00   | 0.1232(23)                       | -0.2638(80)                     | 0.515(33)                       | 0.343(13) | 0.471(81) |
|     | 3.50   | 0.1722(23)                       | -0.2664(83)                     | 0.586(53)                       | 0.461(12) |          |
|     | 3.00   | 0.2381(21)                       | -0.2783(68)                     | 0.737(35)                       | 0.557(85) |          |
|     | 2.70   | 0.2828(19)                       | -0.3107(79)                     | 0.781(34)                       | 0.577(84) |          |
|     | 2.50   | 0.3180(23)                       | -0.3261(74)                     | 0.807(52)                       | 0.598(74) |          |
|     | 2.00   | 0.4183(22)                       | -0.4581(79)                     | 0.846(32)                       | 0.578(57) |          |
|     | 1.70   | 0.4809(24)                       | -0.6166(75)                     | 0.765(56)                       | 0.532(44) | 0.57(12) |
|     | 1.60   | 0.5131(24)                       | -0.7058(79)                     | 0.699(39)                       | 0.5027(42)| 0.723(23)|
|     | 1.50   | 0.5376(22)                       | -0.8143(78)                     | 0.518(37)                       | 0.4689(37)| 0.835(17)|
| 3   | 1.40   | 0.5795(23)                       | -0.8755(76)                     | 0.542(37)                       | 0.4698(34)| 0.839(15)|
|     | 1.20   | 0.6212(22)                       | -1.2529(83)                     | -0.043(39)                      | 0.3648(28)| 1.009(13)|
|     | 1.00   | 0.6518(19)                       | -1.9239(68)                     | -1.139(31)                      | 0.2286(16)| 1.152(11)|
| 5   | 0.80   | 0.6964(34)                       | -3.009(11)                      | -3.277(63)                      | 0.1153(15)| 1.293(24)|
Table 4: The BLM scale for the energy shift $E_0$ for several values of the bare lattice mass $aM_0$ in NRQCD without tadpole improvement. $aq_1^*$ gives the scale set by Eq. (3) in units of the inverse lattice spacing. $aq_2^*$ gives the preferred scale by Eq. (13) where appropriate. The parameter $n$ is set to ensure the stability of heavy quark propagator evolution in simulations [76].

| $n$ | $aM_0$ | $(f) ≡ E_0/\alpha_s$ | $\langle f \log((aq)^2) \rangle$ | $\langle f \log^2((aq)^2) \rangle$ | $aq_1^*$ | $aq_2^*$ |
|-----|--------|----------------------|-------------------------------|---------------------------------|--------|--------|
| 1   | 20.00  | 2.2571(48)           | 2.5490(13)                    | 10.8100(38)                    | 1.75884(55) | –      |
|     | 17.50  | 2.2765(44)           | 2.6011(12)                    | 10.9496(40)                    | 1.77051(52) | –      |
|     | 15.00  | 2.3033(45)           | 2.6694(13)                    | 11.1328(39)                    | 1.78507(54) | –      |
|     | 12.50  | 2.3389(69)           | 2.7653(22)                    | 11.3882(87)                    | 1.80606(92) | –      |
|     | 10.00  | 2.39196(65)          | 2.9062(23)                    | 11.7729(84)                    | 1.83583(92) | –      |
|     | 7.00   | 2.50419(41)          | 3.1988(14)                    | 12.5623(49)                    | 1.89398(57) | –      |
|     | 5.00   | 2.64980(48)          | 3.5784(15)                    | 13.5643(49)                    | 1.96446(59) | –      |
|     | 4.00   | 2.77360(93)          | 3.8955(38)                    | 14.4059(99)                    | 2.0198(15)  | –      |
| 2   | 4.00   | 2.77159(78)          | 3.8981(28)                    | 14.380(11)                     | 2.0203(11)  | –      |
|     | 3.50   | 2.8585(10)           | 4.1118(34)                    | 14.952(11)                     | 2.0529(13)  | –      |
|     | 3.00   | 2.97012(88)          | 4.3973(34)                    | 15.670(12)                     | 2.0965(13)  | –      |
|     | 2.70   | 3.0574(11)           | 4.6137(38)                    | 16.228(11)                     | 2.1266(15)  | –      |
|     | 2.50   | 3.12485(90)          | 4.7822(41)                    | 16.660(12)                     | 2.1494(15)  | –      |
|     | 2.00   | 3.3492(12)           | 5.3483(43)                    | 18.116(15)                     | 2.2221(16)  | –      |
|     | 1.70   | 3.5394(13)           | 5.8316(43)                    | 19.302(14)                     | 2.2791(15)  | –      |
|     | 1.60   | 3.6163(13)           | 6.0299(45)                    | 19.843(16)                     | 2.3018(16)  | –      |
|     | 1.50   | 3.7057(14)           | 6.2486(45)                    | 20.406(17)                     | 2.3236(16)  | –      |
| 3   | 1.40   | 3.7865(16)           | 6.4417(61)                    | 20.873(18)                     | 2.3411(21)  | –      |
|     | 1.20   | 4.0175(17)           | 7.0245(61)                    | 22.344(17)                     | 2.3970(20)  | –      |
|     | 1.00   | 4.32658(96)          | 7.8282(35)                    | 24.418(11)                     | 2.4711(11)  | –      |
| 5   | 0.80   | 4.6581(20)           | 8.7418(74)                    | 26.784(27)                     | 2.5557(23)  | –      |
Table 5: The BLM scale for the energy shift $E_0$ for several values of the bare lattice mass $aM_0$ in NRQCD with tadpole improvement. $aq_1^*$ gives the scale set by Eq. (3) in units of the inverse lattice spacing. $aq_2^*$ gives the preferred scale by Eq. (13) where appropriate. The parameter $n$ is set to ensure the stability of heavy quark propagator evolution in simulations [76].

| $n$ | $aM_0$ | $(f) \equiv E_0/\alpha_s$ | $\langle f \log((aq)^2) \rangle$ | $\langle f \log^2((aq)^2) \rangle$ | $aq_1^*$ | $aq_2^*$ |
|-----|--------|-----------------------------|----------------------------------|----------------------------------|--------|--------|
| 1   | 20.00  | 1.05283(48)                 | -0.3998(13)                      | 3.2048(38)                       | 0.82706(52) | –      |
|     | 17.50  | 1.04985(44)                 | -0.4027(12)                      | 3.2027(40)                       | 0.82549(50) | –      |
|     | 15.00  | 1.04669(45)                 | -0.4076(13)                      | 3.1970(39)                       | 0.82306(51) | –      |
|     | 12.50  | 1.04040(69)                 | -0.4143(22)                      | 3.1878(87)                       | 0.81948(89) | –      |
|     | 10.00  | 1.03060(65)                 | -0.4272(23)                      | 3.1758(84)                       | 0.81281(90) | –      |
|     | 7.00   | 1.00820(41)                 | -0.4643(14)                      | 3.1150(49)                       | 0.79431(56) | –      |
|     | 5.00   | 0.97428(48)                 | -0.5243(15)                      | 2.9833(49)                       | 0.76409(58) | –      |
|     | 4.00   | 0.94100(93)                 | -0.5878(38)                      | 2.8305(99)                       | 0.7318(15)  | –      |
| 2   | 4.00   | 0.93900(78)                 | -0.5891(28)                      | 2.807(11)                        | 0.7307(11)  | –      |
|     | 3.50   | 0.9137(10)                  | -0.6502(34)                      | 2.671(11)                        | 0.7006(13)  | –      |
|     | 3.00   | 0.87572(88)                 | -0.7311(34)                      | 2.444(12)                        | 0.6588(13)  | –      |
|     | 2.70   | 0.8466(11)                  | -0.7996(38)                      | 2.266(11)                        | 0.6236(15)  | –      |
|     | 2.50   | 0.82102(90)                 | -0.8590(41)                      | 2.111(12)                        | 0.5927(15)  | –      |
|     | 2.00   | 0.7312(12)                  | -1.0621(43)                      | 1.583(15)                        | 0.4837(16)  | –      |
|     | 1.70   | 0.6442(13)                  | -1.2576(43)                      | 1.018(14)                        | 0.3768(15)  | 0.7950(59) |
|     | 1.60   | 0.6056(13)                  | -1.3421(45)                      | 0.830(16)                        | 0.3302(14)  | 0.8460(65) |
|     | 1.50   | 0.5641(14)                  | -1.4439(45)                      | 0.566(17)                        | 0.2781(14)  | 0.9029(73) |
| 3   | 1.40   | 0.4953(16)                  | -1.6171(61)                      | 0.088(18)                        | 0.1955(16)  | 0.986(12) |
|     | 1.20   | 0.3523(17)                  | -1.9501(61)                      | -0.802(17)                       | 0.06282(99) | 1.106(24) |
|     | 1.00   | 0.13779(96)                 | -2.4285(35)                      | -2.035(11)                       | 0.0001489(93) | 1.23(11) |
| 5   | 0.80   | -0.3161(20)                 | -3.4380(74)                      | -4.629(27)                       | 230.0(8.4)  | 1.416(75) |
order formula in Eq. (3) applies. The choice of sign for the second-order solution should be apparent either from continuity, or by checking that the solution minimizes the next higher (cubic) moment in Eq. (55) if it is available. In addition, higher moments give a measure of the range $\Delta q$ of momenta which flow through the gluon, and can confirm that the $q^*$ chosen in either case is indeed typical. Large values for the relative range $\Delta q/q$ can indicate large higher-order contributions even when $q^*$ is large.

Our second-order prescription has several advantages. It requires a simple extension to the calculation, either numeric and analytic, needed to implement the first-order prescription, requiring only computation of an additional logarithmic moment. Calculation of higher moments can then help to further characterize the diagram and confirm the scale choice. It can also identify cases where the first two terms are anomalously small, though such cases are apparently rare. It is appropriate regardless of the number of loops included in the running coupling, and is not limited to the strong interactions. Finally, it remedies erroneous scales in a variety of processes.

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