Scale Setting for $\alpha_s$ Beyond Leading Order

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We present a general procedure for applying the scale-setting prescription of Brodsky, Lepage and Mackenzie to higher orders in the strong coupling constant $\alpha_s$. In particular, we show how to apply this prescription when the leading coefficient or coefficients in a series in $\alpha_s$ are anomalously small. 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 find significant corrections to the scales for $R_{e^+e^-}$, $\Gamma(B \to X_u\ell\nu)$, $\Gamma(t \to bW)$, and the ratios of the quark pole to $\overline{MS}$ and lattice bare masses.

1. Introduction

QCD processes computed to a finite order in perturbation theory depend on the scale chosen for the running coupling constant $\alpha_s(q)$. While these variations diminish as higher orders are included, for low-order calculations they can be significant. Finding an optimum, physically motivated method for choosing this scale is important not only to produce accurate results, but also to reasonably estimate convergence based on the size of the series coefficients. Such a method allows a meaningful prediction or comparison with data even at leading order.

In this paper, we apply the prescription defined by Brodsky, Lepage and Mackenzie (BLM) in Refs. \cite{1,2} beyond leading order. In so doing, we remedy an anomaly observed in a variety of applications as discussed, for example, in Ref. \cite{3}. We show that this requires a simple extension of the calculation needed to set the scale at lowest order. We find that it leads to significant corrections in the scales of several important processes, and allows us to extract masses from lattice simulations which were previously inaccessible. (See Refs. \cite{5,6} for other higher-order extensions.)

2. The Prescription

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{The BLM prescription fixing the optimum scale $q^*$ to leading order in $\alpha_s(q^*)$. Vacuum bubbles include both fermions and gluons.}
\end{figure}

The original statement of the prescription,

$$\alpha_s(q^*) \int d^4q f(q) \approx \int d^4q \alpha_s(q)f(q)$$

(1)

illustrated in Fig. \cite{1}, is to choose the scale $q^*$ associated with a particular gluon such that it matches, as well as possible, the same diagram with a fully dressed gluon \cite{1}. Here $f(q)$ is the integrand within the diagram which includes the gluon. In this way, $\alpha_s(q^*)$ absorbs much of the effect of these higher-order corrections, and represents the true strength of this gluon's coupling
to the rest of the diagram. When \( f(q) \) is sensitive to large \( q \), expanding \( \alpha_s \) on both sides at a common scale \( \mu \) gives a form suitable for numerical calculation,

\[
\log(q^2/\mu^2) = \frac{\langle f(q) \log(q^2/\mu^2) \rangle}{\langle f(q) \rangle} \equiv \langle \log(q^2/\mu^2) \rangle, \tag{2}
\]

with \( q^* \) given by the average log of the momentum running through that gluon [3].

3. The Problem

When \( \langle f(q) \rangle \) vanishes, Eq. (2) is meaningless. Even when nonzero, if \( \langle f(q) \rangle \) is anomalously small compared to \( \langle f(q) \log(q^2/\mu^2) \rangle \), the result can be misleading. This occurs in a variety of processes, and for some set of parameters in most processes. For example, it occurs for the perturbative relation between the bare lattice quark mass in NRQCD and its pole mass at the value relevant for charm. A gluonic contribution for which \( \langle f(q) \rangle \rightarrow 0 \) is dominated by its second-order term; Eq. (2) fails because it attempts to match a first-order statement of the general prescription to a process which is properly second-order.

4. The Solution

The solution is to apply the prescription beyond leading order, as illustrated in Fig. 2. This gives a reasonable \( q^* \) when the leading diagram is anomalously small, and it approaches a sensible limit when it vanishes altogether. In rare cases when both the first and second order contributions are small, it is simple to carry this one loop higher.

The result of matching at a common scale \( \mu \) is [4]

\[
\log(q^2/\mu^2) = \langle \log(q^2/\mu^2) \rangle \pm \left[ -\sigma^2 \right]^{1/2}, \tag{3}
\]

with

\[
\sigma^2 \equiv \langle \log^2(q^2/\mu^2) \rangle - \langle \log(q^2/\mu^2) \rangle^2. \tag{4}
\]

When \( f(q) \) does not change sign, it may be interpreted as a probability distribution, so \( \sigma^2 > 0 \), and Eq. (3) gives the correct scale. However, when \( \sigma^2 < 0 \), there are evidently significant sign changes, and \( \langle f \rangle \) will be anomalously small. In this case, Eq. (3) gives the correct choice of scale. It causes the leading-order discrepancy between the left and right sides in Fig. 2 to vanish, and minimizes it at next order [3]. Applying Eq. (3) requires only the additional computation of the average log squared within the same integrand as in Eq. (2).

5. A Simple Example

Consider as a simple model for the integrand

\[
f(q) = (1 + c)\delta(q - q_a) - \delta(q - q_b), \tag{5}
\]

tsensitive to two scales, \( q_a \) and \( q_b \). It suffers from partial cancellations when \( c > -1 \), and \( \sigma^2 \) becomes negative; when \( c = 0 \), \( f(q) \) vanishes identically and Eq. (3) blows up. In Fig. 3 we show the result of applying Eq. (3) in this region, and Eq. (3) when \( c < -1 \) and \( \sigma^2 > 0 \). It clearly behaves as expected, with \( q^* \) approaching \( q_a \) when \( |c| \gg 1, q_b \) when \( c = -1 \), remaining between in the interim. Even in the region where \( c \) is large and positive and Eq. (3) gives a well-behaved \( q^* \), Eq. (3) is clearly preferable.

6. Determining \( q^* \) in \( \overline{\text{MS}} \)

The \( g\phi^3 \) self-energy diagram illustrated in Fig. 4 presents a more realistic example. Evaluating the diagram with an additional denominator

\[
g^2 \int \frac{d^nk}{(2\pi)^n} \frac{1}{k^2 + m^2} \frac{1}{(p - k)^2 + m^2} \frac{1}{(k^2/\mu^2)^2}, \tag{6}
\]
Figure 3. The BLM scale $q^*$ as a function of $c$, with $q_a = 2.0$ and $q_b = 1.8$. The first order solution determines $q^*$ for $c < -1$, second order for $c > -1$. Dark dotted lines show the first-order solution in regions in which it does not apply; light dotted lines display inapplicable second-order solutions.

and expanding the result in $\beta$ produces the sequence of average logs needed to set the scale to any desired order. This is not much more difficult within dimensional regularization than computing the diagram itself. In Fig. 5 we display the result for $q^*$ as a function of the propagator momentum $p/m[4]$. The second-order solution is appropriate in the intermediate region. It gives a physically reasonable result which connects continuously with the first-order solution appropriate for large and small $p/m$, whereas the first-order solution diverges in this region.

7. Determining $q^*$ from an Existing Series

When the terms in a series are already known, the average logs needed for scale setting can be extracted by using the dependence on the number of flavors $n_f$, or equivalently, $\beta_0 \equiv (11 - (2/3)n_f)/4\pi$. Contributions from a particular dressed gluon within a diagram take the form

$$c_0\alpha_s(\mu) + (a_1 - c_1\beta_0)\alpha_s^2(\mu) + (a_2 + \cdots + c_2\beta_0^2)\alpha_s^3(\mu) + \cdots. \quad (7)$$

The highest power $n$ of $\beta_0$ at each order in $\alpha_s$ is due to $n$ one-loop vacuum polarization diagrams, and so at large $q$ we may make the identification

$$c_0 = \langle f \rangle$$
$$c_1/c_0 \approx \langle \log(q^2/\mu^2) \rangle$$
$$c_2/c_0 \approx \langle \log^2(q^2/\mu^2) \rangle,$$

allowing us to apply second-order scale setting for a series known to $\alpha_s^3$. Below we use this to present several processes for which Eq. (8) gives the appropriate scale.
8. Higher orders

The series coefficients from a single dressed gluon depend on the scale $q^*$ according to [4]

$$\langle f \rangle \left\{ \alpha_s(q^*) + \alpha_s^2(q^*)[\beta_0 \Delta_1] + \alpha_s^3(q^*)[\beta_0^2 \Delta_2 + \beta_1 \Delta_1] + \alpha_s^4(q^*)[\beta_0^3 \Delta_3 + \frac{5}{2} \beta_0 \beta_1 \Delta_2 + \beta_2 \Delta_1] + \alpha_s^5(q^*)[\beta_0^4 \Delta_4 + \frac{13}{3} \beta_0^2 \beta_1 \Delta_3 + 3 \beta_0 \beta_2 \Delta_2 + \frac{3}{2} \beta_1^2 \Delta_2 + \beta_3 \Delta_1] + \cdots \right\}, \quad (9)$$

with

$$\Delta_n \equiv \langle [\log(q^{*2}/\mu^2) - \log(q^2/\mu^2)]^n \rangle. \quad (10)$$

In this form, the objective in choosing an optimum scale is transparent, regardless of the number of loops kept in $\alpha_s$. For a gluon sensitive to a narrow, large momentum region, choosing the correct $q^*$ will approximately minimize the moments in Eq. (10). Contributions from the higher order diagrams which dress that gluon will be small, having been largely absorbed into the leading term. However, when the region of sensitivity in momentum is large, these moments will be minimized less effectively by a single scale $q^*$, and higher order contributions will be larger.

The general prescription to any order is then to skip any leading terms which are anomalously small, which will rarely be other than the first; choose the $q^*$ which eliminates the coefficient after the first nonanomalous term and minimizes the next; and use higher moments when available to check the consistency of the scale choice.

In Fig. 6 we display the dependence of these moments on $\log(q^{*2}/\mu^2)$ for the semileptonic decay width $\Gamma(B \to X_u e\nu_e)$ expressed in terms of the $\overline{\text{MS}}$ mass $M$, using results from Ref. [6]. In this case, Eq. (3) gives the appropriate scale, and examination of the higher moments confirms this. Choosing the second-order prescription eliminates the second moment, minimizes the third moment, and $\log(q^{*2})$ is near either the zero or minimum for all the higher moments. As a result, higher order coefficients are small, and the leading term effectively represents the strength of this gluon’s coupling.

9. Applications

When at least the second logarithmic moment is available, we may apply scale setting beyond leading order. Ref. [2] presents a collection of such series. In Table 1, we list results for four of these for which Eq. (3) gives the appropriate scale: $R_{e^+e^-}$, the ratio of the pole to $\overline{\text{MS}}$ mass $M/\overline{\text{M}}$, and the $B$ and $t$ decay widths $\Gamma(B \to X_u e\nu_e)$ and $\Gamma(t \to bW)$ expressed in terms of $\overline{\text{MS}}$ masses. These new scales represent significant corrections to the scales set by Eq. (2). While the new scale for $M/\overline{\text{M}}$ is increased, we note that the range of important momenta $\Delta q$ is still relatively large, indicating sensitivity to low-momentum scales even when $M$ is large, and threatening growing higher-order coefficients. This is not the case for $B$ and $t$ decays provided their series are expressed in terms of the short-distance $\overline{\text{MS}}$ masses, as indi-
Table 1
Applications of second-order scale setting to several processes. $q_1$ gives the scale set by Eq. (2); $q_2$ gives the preferred scale by Eq. (3). $\Delta q$, measures the range of momentum running through the gluon $q$.

| $c_1/c_0$ | $q_1^*$ | $c_2/c_0$ | $\sigma^2$ | $q_2^*$ | $\Delta q$ |
|-----------|---------|-----------|------------|---------|-----------|
| $\frac{R_{e^+e^-}(s)}{M/M}$ | $-0.691772$ | $0.7076\sqrt{s}$ | $-0.186421$ | $-0.664971$ | $1.064\sqrt{s}$ | $-$ |
| $\Gamma(B \to X_u e\bar{\nu})/M_b^3$ | $-4.6862$ | $0.09603M$ | $17.623$ | $-4.3374$ | $0.27205M$ | $0.38M$ |
| $\Gamma(t \to bW)/M_t^3$ | $-4.3163$ | $0.11554M_b$ | $8.0992$ | $-10.531$ | $0.58534M_b$ | $0.35M_b$ |
| $-5.7076$ | $0.05763M_t$ | $6.0996$ | $-26.477$ | $0.75502M_t$ | $0.34M_t$ |

In Fig. 7, we show the scale associated with the series connecting the quark pole mass to the NRQCD lattice bare mass. At both small and large values of the bare mass, Eq. (3) is appropriate and necessary to give an accurate measure of the optimum scale.

10. Conclusions

We have presented a simple general procedure for applying BLM scale-setting beyond leading order. Our main result is the second-order prescription Eq. (3), which is appropriate when the leading contribution is anomalously small. We gave a general method for computing an optimum scale numerically, within dimensional regularization, and in cases when the coefficients of a series are known, and applied it to several processes. Finally, we discussed its application at higher orders.

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