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Setting the Renormalization Scale in QCD: The Principle of Maximum Conformality

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A key problem in making precise perturbative QCD predictions is the uncertainty in determining the renormalization scale μ of the running coupling $\alpha_s(\mu^2)$. The purpose of the running coupling in any gauge theory is to sum all terms involving the β function; in fact, when the renormalization scale is set properly, all non-conformal $\beta \neq 0$ terms in a perturbative expansion arising from renormalization are summed into the running coupling. The remaining terms in the perturbative series are then identical to that of a conformal theory; i.e., the corresponding theory with $\beta = 0$. The resulting scale-fixed predictions using the "principle of maximum conformality" (PMC) are independent of the choice of renormalization scheme – a key requirement of renormalization group invariance. The results avoid renormalon resummation and agree with QED scale-setting in the Abelian limit. The PMC is also the theoretical principle underlying the BLM procedure, commensurate scale relations between observables, and the scale-setting method used in lattice gauge theory. The number of active flavors n_f in the QCD β function is also correctly determined. We discuss several methods for determining the PMC/BLM scale for QCD processes. We show that a single global PMC scale, valid at leading order, can be derived from basic properties of the perturbative QCD cross section. The elimination of the renormalization scheme ambiguity using the PMC will not only increase the precision of QCD tests, but it will also increase the sensitivity of collider experiments to new physics beyond the Standard Model.

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I. INTRODUCTION

A key difficulty in making precise perturbative QCD predictions is the uncertainty in determining the renormalization scale μ of the running coupling $\alpha_s(\mu^2)$. It is common practice to simply guess a physical scale $\mu = Q$ of order of a typical momentum transfer Q in the process, and then vary the scale over a range $Q/2$ and $2Q$. This procedure is clearly problematic since the resulting fixed-order pQCD prediction will depend on the choice of renormalization scheme; it can even predict negative QCD cross sections at next-to-leading-order [1].

The purpose of the running coupling in any gauge theory is to sum all terms involving the β function; in fact, when the renormalization scale μ is set properly, all non-conformal $\beta \neq 0$ terms in a perturbative expansion arising from renormalization are summed into the running coupling. The remaining terms in the perturbative series are then identical to that of a conformal theory; i.e., the theory with $\beta = 0$. The divergent "renormalon" series of order $\alpha_s^n \beta^n n!$ does not appear in the conformal series. Thus as in quantum electrodynamics, the renormalization scale μ is determined unambiguously by the "Principle of Maximal Conformality (PMC)". This is also the principle underlying BLM scale setting [2]

It should be recalled that there is no ambiguity in setting the renormalization scale in QED. In the standard Gell-Mann–Low scheme for QED, the renormalization scale is simply the virtuality of the virtual photon [3]. For example, in electron-muon elastic scattering, the renormalization scale is the virtuality of the exchanged photon, spacelike momentum transfer squared $\mu^2 = q^2 = t$. Thus

$$\alpha(t) = \frac{\alpha(t_0)}{1 - \Pi(t, t_0)} \tag{1}$$

where

$$\Pi(t, t_0) = \frac{\Pi(t) - \Pi(t_0)}{1 - \Pi(t_0)} \tag{2}$$

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sums **all** vacuum polarization contributions to the dressed photon propagator, both proper and improper. (Here $\Pi(t) = \Pi(t,0)$ is the sum of proper vacuum polarization insertions, subtracted at $t = 0$). Formally, one can choose any initial renormalization scale $\mu_0^2 = t_0$, since the final result when summed to all orders will be independent of t_0. This is the invariance principle used to derive renormalization group results such as the Callan-Symanzik equations [4, 5]. However, the formal invariance of physical results under changes in t_0 does not imply that there is no optimal scale. In fact, as seen in QED, the scale choice $\mu^2 = q^2$, the photon virtuality, immediately sums all vacuum polarization contributions to all orders exactly. With any other choice of scale, one will recover the same result, but only after summing an infinite number of vacuum polarization corrections.

Thus, although the *initial* choice of renormalization scale t_0 is arbitrary, the *final* scale t which sums the vacuum polarization corrections is unique and unambiguous. The resulting perturbative series is identical to the conformal series with zero β-function. In the case of muonic atoms, the modified muon-nucleus Coulomb potential is precisely $-Z\alpha(-\vec{q}^{\,2})/\vec{q}^{\,2}$; i.e., $\mu^2 = -\vec{q}^2$. Again, the renormalization scale is unique.

One can employ other renormalization schemes in QED, such as the $\overline{MS}$ scheme, but the physical result will be the same once one allows for the relative displacement of the scales of each scheme. For example, one can compute the standard one-loop charged lepton pair vacuum polarization contribution to the photon propagator at photon virtuality q^2 using dimensional regularization. The result in $\overline{MS}$ scheme for spacelike argument $q^2 = -Q^2$ is

$$\log \frac{\mu^2_{\overline{MS}}}{m_\ell^2} = 6 \int_0^1 x(1-x) \log \frac{m_\ell^2 + Q^2 x(1-x)}{m_\ell^2}. \tag{3}$$

At large Q^2 this is

$$\log \frac{\mu^2_{\overline{MS}}}{m_\ell^2} = \log \frac{Q_0^2}{m_\ell^2} - 5/3; \tag{4}$$

i.e., $\mu^2_{\overline{MS}} = Q^2 e^{-5/3}$. Thus if $Q^2 >> 4m_\ell^2$, we can identify

$$\alpha_{\overline{MS}}(e^{-5/3}q^2) = \alpha_{GM-L}(q^2). \tag{5}$$

The $e^{-5/3}$ displacement of renormalization scales between the $\overline{MS}$ and Gell-Mann–Low schemes is a result of the convention [6] which was chosen to define the minimal dimensional regularization scheme. One can use another definition of the renormalization scheme, but the final physical prediction cannot depend on the convention. This invariance under choice of scheme is a consequence of the transitivity property of the renormalization group [3, 7–9].

The same principle underlying renormalization scale-setting in QED must also hold in QCD since the n_F terms in the QCD β function have the same role as the lepton N_ℓ vacuum polarization contributions in QED. QCD and QED share the same Yang-Mills Lagrangian. In fact, one can show [10] that QCD analytically continues as a function of N_C to Abelian theory when $N_C \to 0$ at fixed $\alpha = C_F \alpha_s$ with $C_F = \frac{N_C^2-1}{2N_C}$. For example, at lowest order $\beta_0^{QCD} = \frac{11}{3}N_C - \frac{2}{3}n_F \to -\frac{2}{3}n_F$ at $N_C = 0$. Thus the same scale-setting procedure must be applicable to all renormalizable gauge theories.

Thus there is a close correspondence between the QCD renormalization scale and that of the analogous QED process. For example, in the case of e^+e^- annihilation to three jets, the PMC/BLM scale is set by the gluon jet virtuality, just as in the corresponding QED reaction. The specific argument of the running coupling depends on the renormalization scheme because of their intrinsic definitions; however, the actual numerical prediction is scheme-independent.

The basic procedure for PMC/BLM scale setting is to shift the renormalization scale so that all terms involving the β function are absorbed into the running coupling. The remaining series is then identical with a conformal theory with $\beta = 0$. Thus, an important feature of the PMC is that its QCD predictions are independent of the choice of renormalization scheme. The PMC procedure also agrees with QED in the $N_C \to 0$ limit.

The determination of the PMC-scale for exclusive processes is often straightforward. For example, consider the process $e^+e^- \to c\bar{c} \to c\bar{c}g^* \to c\bar{c}b\bar{b}$, where all the flavors and momenta of the final-state quarks are identified. The n_f terms at NLO come from the quark loop in the gluon propagator. Thus the PMC scale for the differential cross section in the $\overline{MS}$ scheme is given simply by the $\overline{MS}$ scheme displacement of the gluon virtuality: $\mu^2_{PMC} = e^{-5/3}(p_b + p_{\bar{b}})^2$.

In practice, one can identify the PMC/BLM scale for QCD by varying the initial renormalization scale μ_0^2 to identify all of the β-dependent nonconformal contributions. At lowest order $\beta_0 = 11/3N_C - 2/3n_F$. Thus at NLO one can simply use the dependence on the number of flavors n_f which arises from the quark loops associated with ultraviolet renormalization as a marker for β_0. Of course in QCD, the n_F terms arise from the renormalization if the three-gluon and four-gluon vertices as well as from gluon wavefunction renormalization.

It is often stated that the argument of the coupling in a renormalization scheme based on dimensional regularization has no physical meaning since the scale μ was originally introduced as a mass parameter in extended space-time dimensions. However, the QED example above shows that the $\overline{MS}$ scale is unambiguously related to invariants in physical 3+1 space. The connection of $\alpha_{\overline{MS}}$ to the Gell-Mann–Low scheme can be established at all orders. This also provides the analytic extension [11] of the $\alpha_{\overline{MS}}$ scheme for finite fermion masses as well to timelike arguments where the coupling is complex.

The PMC/BLM scale which appears in the three-gluon vertex is a function of the virtuality of the three external gluons q_1^2, q_2^2, and q_3^2. It has been computed in detail in refs. [12]. The results are surprising when the virtualities are very different as in the subprocess $gg \to g \to Q\bar{Q}$.

$$\hat{\mu}^2 \propto \frac{q^2_{\rm min} q^2_{\rm med}}{q^2_{\rm max}} \tag{6}$$

where $|q^2_{\rm min}| < |q^2_{\rm med}| < |q^2_{\rm max}|$; i.e. $q^2_{\rm max}$ has the **maximal** virtuality [13]. The same scale also correctly sets the effective number of quarks n_f which appear in the β function controlling the three-gluon vertex renormalization. This example shows that it is critical to properly fix the renormalization scale; a prediction based on guessing that $\mu^2 \simeq q^2_{max}$ will give misleading results.

It is sometimes argued that it is advantageous not to fix the renormalization scale at all, since its variation provides a measure of higher order contributions to the theory predictions. In fact, one obtains sensitivity only to the β-dependent non-conformal terms by this procedure. In some cases the conformal contributions may be unexpectedly large. For example, the very large electron-loop light-by-light scattering contribution [14] $\simeq 18(\alpha^3/\pi)^3$ to the muon anomalous magnetic moment is unassociated with renormalization or the β function. Of course, one can still compute the variation of the prediction around the PMC scale as an indicator of higher order non-conformal terms.

Stevenson has proposed that one should set the renormalization scale at a point where the predicted cross section has minimal variation with respect to μ – the "principle of minimal sensitivity" (PMS) [15]. However, unlike the PMC, the application of the PMS to jet production gives unphysical results [16] since it sums physics into the running coupling not associated with renormalization. Worse, the PMS prediction depends on the choice of renormalization scheme, and it violates the transitivity property of the renormalization group [17]. Such heuristic scale-setting methods also give incorrect results when applied to Abelian QED.

It should be emphasized that the *factorization scale* which enters predictions for QCD inclusive reactions is introduced to match nonperturbative and perturbative aspects of the parton distributions in hadrons; it is present even in conformal theory, and thus its determination is a completely separate issue from *renormalization scale* setting.

II. IDENTIFYING THE RENORMALIZATION SCALE USING THE PRINCIPLE OF MAXIMUM CONFORMALITY

Given the analytic form of the hard process amplitude or cross section as a series in $\alpha_s(\mu_0^2)$ evaluated at an initial scale μ_0^2, one can identify the PMC scale in a systematic way:

1. The variation of the cross section with respect to $\log \mu_0^2$ can be used to distinguish the conformal terms versus the nonconformal terms proportional to the β function.

2. The identified nonconformal terms have the form $\beta \times \log p_{ij}/\mu_0^2$ where $p_{ij} = p_i \cdot p_j$ are the scalar product invariants $i \neq j$ which enter the hard subprocess. In practice, these terms can be identified as coefficients of n_f, the number of flavors appearing in the β function; i.e., the flavor dependence arising from quark loops associated with coupling constant renormalization. The n_F terms in QCD arise from the renormalization if the three-gluon and four-gluon vertices as well as from gluon wavefunction renormalization.

3. The scale is then shifted $\mu_0^2 \to \hat{\mu}^2$ in order to absorb the non-conformal terms. Thus when the scale is correctly set, the coefficients of $\alpha_s(\mu^2)$ become independent of the β function and $\log \hat{\mu}^2$.

4. The series is then identical to that of the conformal theory where $\beta = 0$ as given by the Banks-Zaks method [18].

   Other examples of this procedure will be given in the next sections.

A. The Global PMC Scale

Ideally, as in the BLM method, one should allow for separate scales for each skeleton graph; e.g., for electron-electron scattering, one takes $\alpha(t)$ and $\alpha(u)$ for the t-channel and u-channel amplitudes, respectively.

Setting separate renormalization scales can be a challenging task for complicated processes in QCD where there are many final-state particles and thus many possible Lorentz scalars $p_{ij}^2 = p_i \cdot p_j$. However, one can obtain a useful first approximation to the full PMC/BLM scale-setting procedure by using a single *global* scale $\hat{\mu}^2$ which appropriately weights the individual BLM scales.

The global scale can be determined by varying the subprocess amplitude with respect to each invariant, thus determining the coefficients f_{ij} of $\log p_{ij}^2/\mu_0^2$ in the nonconformal terms in the amplitude. The global PMC scale is then

$$\hat{\mu}^2 = C \times \Pi_{ij}\ [p_{ij}^2]^{w_{ij}}, \tag{7}$$

i.e.,

$$\log \hat{\mu}^2 = \sum_{i \neq j} w_{ij} \log p_{ij}^2 + \log C \tag{8}$$

where the weight for each invariant is

$$w_{ij} = \frac{f_{ij}}{\sum_{i \neq j} f_{ij}}. \tag{9}$$

and $\sum_{i \neq j} w_{ij} = 1$. The constant C is the scheme displacement; e.g., $C = e^{-5/3}$ for $\overline{MS}$ for $\hat{\mu}^2 >> 4m_f^2$.

As a specific example of the application of a PMC global scale, consider the electron-electron scattering amplitude in QED. (For simplicity, we will just take the contribution of the convection current to the amplitude, as in scalar QED.) The Lorentz invariant Born amplitude is then

$$M^0(t,u) = 4\pi\alpha_0\big(\frac{s-u}{t} + \frac{s-t}{u}\big). \tag{10}$$

The running QED coupling $\alpha(q^2)$ in QED sums all proper and improper vacuum polarization graphs

$$M(t,u) = 4\pi\alpha(t)\big(\frac{s-u}{t}\big) + 4\pi\alpha(u)\big(\frac{s-t}{u}\big) \tag{11}$$

where to leading order

$$\alpha(t) = \alpha(t_0)\big(1 + n_\ell \frac{\alpha(t_0)}{3\pi} \log \frac{-t}{t_0}\big). \tag{12}$$

Aside from power-suppressed contributions involving the lepton masses, the resulting series is identical to the corresponding conformal theory with $\beta = 0$.

In this process we have contributions from both the t - and u- channel amplitudes which require separate renormalization scales for each skeleton graph. However, at leading order we can weight the amplitudes to obtain a single PMC/BLM scale which still sums the nonconformal β terms into the running coupling $\alpha(\mu^2)$ at leading order. For example, using the standard Gell-Mann–Low scheme, we can write

$$M(t,u) = f(t)\alpha(t) + g(u)\alpha(u) = (f(t) + g(u))\alpha(\hat{\mu}^2) \tag{13}$$

where $f(t) = 4\pi(s-u)/t$ and $g(u) = 4\pi(s-t)/u$ are the Born amplitudes for the t - and u -channels, respectively.

The logarithm of the global scale is then

$$\log \hat{\mu}^2 = \frac{f(t)}{f(t)+g(u)} \log(-t) + \frac{g(u)}{f(t)+g(u)} \log(-u) \tag{14}$$

which duplicates the multi-scale result at NLO. Using kinematical constraints such as the total momentum conservation $s+t+u = 0$ the weighted scale dependence can be confined into the $\log(t/u)$ term inside the running coupling. The global scale $\hat{\mu}^2$ is maximal at $\theta_{CM} = \pi/2$ ($\mu^2 = \sqrt{tu} = -t = -u$) and vanishes at the boundaries $(0,\pi)$ where $\tan^2(\theta_{CM}/2) = t/u$. The results are shown in Fig. 1.

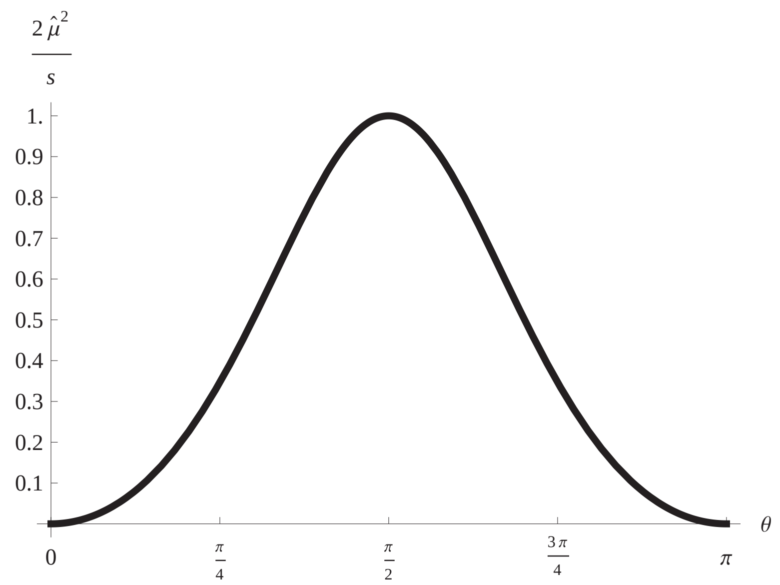

FIG. 1: The PMC/BLM scale as function of the CM angle θ_{CM}:$e\,e \rightarrow e\,e$ scalar QED

III. A PMC EXAMPLE FOR QCD: APPLICATION TO JET CROSS SECTIONS IN ELECTRON-POSITRON ANNIHILATION

As an example of the application of the PMC to QCD, we will show how the renormalization scale can be determined for the cross sections for e^+e^- annihilation into two, three and four jets in $\overline{MS}$ scheme.

The two-jet cross section has only infrared divergences:

$$\sigma^{(2)} = \sigma_0\Big(\frac{4\pi\mu^2}{q^2}\Big)^{\lambda/2}\big(1-\lambda/2\big)\frac{\Gamma(1-\lambda/2)}{\Gamma(2-\lambda)} \tag{15}$$

where $\sigma_0 = 4\pi\frac{\alpha^2}{3q^2}N_C\sum_{i=1}^{N_f}e_i^2$.

Here $\lambda \equiv 4-n$ is the number of extra space-time dimensions used to regulate infrared and ultraviolet divergent integrals. Eventually all of the infrared divergences and the factors involving λ will cancel out. In dimensional regularization the scale μ is introduced as a mass scale to restore the correct dimension of the coupling. The gauge coupling g_R is related to the renormalized coupling constant α_R by

$$\frac{g_R^2}{(4\pi)^{(4-\lambda)/2}} = \frac{\alpha_s(\mu^2)}{4\pi}(\mu^2)^{\lambda/2}e^{\gamma_E\lambda/2} \tag{16}$$

and here γ_E is the Euler constant.

As discussed in the introduction, the mass scale of schemes defined by dimensional regularization attains its physical meaning when it is applied to QED. The renormalized gauge coupling is also related to the bare coupling by:

$$g_R = \sqrt{Z_3}Z_2/Z_1 g_0, \tag{17}$$

where Z_1 is the renormalization constant for the quark-antiquark-gluon vertex, Z_2 for the quark field and Z_3 for the gluon field. The renormalization constants are:

$$Z_1 = 1-\frac{g_0^2}{16\pi^2}\,(N_c+C_F)\left(\frac{2}{\lambda_{UV}}-\frac{2}{\lambda_{IR}}\right) \tag{18}$$

$$Z_2 = 1-\frac{g_0^2}{16\pi^2}\,C_F\left(\frac{2}{\lambda_{UV}}-\frac{2}{\lambda_{IR}}\right) \tag{19}$$

$$Z_3 = 1+\frac{g_0^2}{16\pi^2}\,(\frac{5}{3}N_c-\frac{2}{3}N_f)\left(\frac{2}{\lambda_{UV}}-\frac{2}{\lambda_{IR}}\right) \tag{20}$$

$$\tag{21}$$

where λ_{UV}, λ_{IR} are related respectively to the $UV-$ultraviolet and $IR-$infrared poles. In the MS only the pole associated with UV renormalization is subtracted out, and this leads us to a redefinition of the gauge coupling:

$$\frac{1}{g_R}\,\delta g_0 = \frac{g_R^2}{16\pi^2}(\frac{2}{3}N_f - \frac{11}{3}N_c)\,\frac{1}{\lambda_{UV}} \tag{22}$$

A suitable renormalization scheme is the $\overline{MS}$ which differs from MS by a constant term and the respective counterterm can be inserted in the Born cross section by shifting the coupling constant:

$$\alpha_s^0 = \alpha_s^{\overline{MS}}\left\{1 - \left(\frac{11}{6}N_c - \frac{2}{3}T_R\right)\frac{\alpha_s^{\overline{MS}}}{2\pi}\left(\frac{1}{\epsilon} + (\ln 4\pi - \gamma_E)\right)\right\} = \alpha_s^{\overline{MS}}\left\{1 - \beta_0\alpha_s^{\overline{MS}}\left(\frac{1}{\bar{\epsilon}}\right)\right\} \tag{23}$$

where:

$$\frac{1}{\bar{\epsilon}} = \frac{1}{\epsilon} + (\ln 4\pi - \gamma_E), \tag{24}$$

$$\beta_0 = \frac{1}{2\pi}\left(\frac{11}{6}N_c - \frac{2}{3}T_R\right) \tag{25}$$

with $T_R = N_f/2\,,\ \epsilon = \lambda_{UV}/2$.

The Born cross section for $e^+e^- \to q(p_1)\bar{q}(p_2)g(p_3)$ for massless quarks and gluons is

$$\left.\frac{d\sigma^{(3)}(\mu^2)}{dx_1dx_2}\right|_{\text{Born}} = \sigma^{(2)}\ (\frac{4\pi\mu^2}{q^2})^{\lambda/2}\ \frac{1}{\Gamma(1-\lambda/2)}\,F_\lambda(x_1,x_2)\,\frac{\alpha_s^{MS}(\mu^2)}{2\pi}\ C_F B^{V-\lambda/2S}(x_1,x_2) \tag{26}$$

Here

$$F_\lambda(x_1,x_2) = [(x_1+x_2-1)(1-x_1)(1-x_2)]^{-\lambda/2} \tag{27}$$

and

$$B^{V-\lambda/2S}(x_1,x_2) = B^V(x_1,x_2) - \frac{\lambda}{2}B^S(x_1,x_2) \tag{28}$$

$$B^V(x_1,x_2) = \frac{x_1^2+x_2^2}{(1-x_1)(1-x_2)} \tag{29}$$

$$B^S(x_1,x_2) = \frac{x_3^2}{(1-x_1)(1-x_2)} \tag{30}$$

where $x_i = \frac{2E_i}{\sqrt{q^2}}$ in the e^+e^- CM. In terms of invariants: $y_{ij} = s_{ij}/q^2 = (p_i+p_j)^2/q^2$. Then $x_1 = 1 - y_{23}, x_2 = 1 - y_{13}, x_3 = 1 - y_{12}, x_1 + x_2 + x_3 = 2$.

The renormalized one-loop corrected cross section for $e^+e^- \to q(p_1)\bar{q}(p_2)g(p_3)$ is given by Eq. (2.11) of Fabricius et al. [21] For our purposes it is sufficient to quote only the term proportional to β_0 in the $\overline{MS}-$scheme:

$$\left.\frac{d\sigma^{(3)}}{dx_1dx_2}\right|_{\text{oneloop}} = \left.\frac{d\sigma^{(3)}(\mu^2)}{dx_1dx_2}\right|_{\text{Born}}\ \left[1 + \alpha_s(\mu^2)\frac{\Gamma(1-\lambda/2)}{\Gamma(1-\lambda)}(\frac{4\pi\mu^2}{q^2})^{\lambda/2}\ \beta_0\big(\log\frac{\mu^2}{q^2}\big) + \cdots\right] \tag{31}$$

where the coupling is defined as in Eq. 23: $\alpha_{MS}(e^{\log 4\pi - \gamma_E}\mu^2) \equiv \alpha_{\overline{MS}}(\mu^2)$. The remaining contributions are independent of N_F and β_0

We can eliminate the non-conformal log-term proportional to β_0 by shifting the renormalization scale $\alpha_{MS}(\mu^2)$ in the Born cross section Eq. 26

$$\alpha_s(\mu^2)\ \simeq\ \alpha_s(q^2)\left(1 - \alpha_s(q^2)\,\beta_0\ \log[\frac{\mu^2}{q^2}]\right);$$

however, it is first convenient to shift the scale to $\mu^2 \to (\mu_0^2)$. Then

$$\left.\frac{d\sigma^{(3)}}{dx_1dx_2}\right|_{\text{oneloop}} = \left.\frac{d\sigma^{(3)}(\mu_0^2)}{dx_1dx_2}\right|_{\text{Born}}\ \left[1 + \alpha_s(\mu_0^2)\frac{\Gamma(1-\lambda/2)}{\Gamma(1-\lambda)}(\frac{4\pi\mu_0^2}{q^2})^{\lambda/2}\ \beta_0\big(\log\frac{\mu_0^2}{q^2}\big) + \cdots\right] \tag{32}$$

Naively one could simply fix the scale to $\sqrt{q^2}$, but the 3-jet cross section will still be affected by IR divergences; in order to apply the PMC/BLM prescription we will first need to include the 4-jet contributions.

IV. NUMERICAL SCALE FIXING

The complete differential 3-jet cross section has been calculated by Fabricius et al. [21], and we quote here the results for the β_0-dependent terms:

$$\frac{d^2\sigma^{(3)}(\epsilon,\delta)}{dx_1 dx_2} = \sigma_0 \frac{\alpha_s(q^2)}{2\pi} C_F \times \tag{33}$$

$$\left\{ B^V(x_1,x_2) \left[1 - \alpha_s(q^2)\ \beta_0\ \left(\log(\frac{1-\ \cos\delta}{2}) +\ \log \hat{x}_3^2 - \ \frac{13}{3} \right) \right] - B^S(x_1,x_2)\,\alpha_s(q^2)\,\frac{\beta_0}{2} \right\} + \mathcal{O}(\delta^2)) + \cdots \tag{34}$$

where $\hat{x}_3 = (2 - x_1 - x_2)$ and

$$d\sigma^{(3)}(\epsilon,\delta) = d\sigma^{(3)} + d\sigma^{(4)}(\epsilon,\delta) \tag{35}$$

is the sum of the 3- and the 4-jets contributions. The cancellation of the IR-poles is guaranteed by the KLN theorem [19, 20].

The variables (ϵ,δ) are small quantities introduced in the virtual amplitude in order to define the soft and collinear 4-jet→3-jet limit (for more details, see Ref. [21]).

In order to extract the PMC/BLM scale we first work in the $\overline{MS}$-scheme, fixing an arbitrary renormalization scale: $\mu^2 = \mu_0^2$. It turns out that β_0 term of the 3-jet differential IR safe cross section has the form:

$$\begin{aligned} \frac{d^2\sigma^{(3)}(\epsilon,\delta)}{dx_1 dx_2} &= \sigma_0 \frac{\alpha_s(\mu_0^2)}{2\pi} C_F \times \\ & \left\{ B^V(x_1,x_2) \left[1 - \alpha_s(\mu_0^2)\,\beta_0\ \left(\log(\frac{1-\cos\delta}{2}) + 2\,\log{(2-x_1-x_2)} - \frac{13}{3} + \log\frac{q^2}{\mu_0^2} \right) \right] + \right. \\ & \left. - B^S(x_1,x_2)\alpha_s(\mu_0^2)\frac{\beta_0}{2} \right\} + \mathcal{O}(\delta^2)) + \cdots . \end{aligned} \tag{36}$$

In principle we can extract information on the terms in this formula performing a detailed analysis of the dependence of the β_0-coefficient on the invariants. Performing a blindfold study we can single out the β_0-coefficient by means of the β_0-derivative of the whole cross section:

$$\begin{aligned} \frac{d}{d\beta_0}\frac{d^2\sigma^{(3)}(\epsilon,\delta)}{dx_1 dx_2} &= \sigma_0 \frac{\alpha_s(\mu_0^2)}{2\pi} C_F \times \\ & \left[B^V(x_1,x_2) \left[-\alpha_s(\mu_0^2)\ \left(\log(\frac{1-\cos\delta}{2}) + 2\,\log{(2-x_1-x_2)}) - \frac{13}{3} + \log\frac{q^2}{\mu_0^2} \right) \right] + \right. \\ & \left. - B^S(x_1,x_2)\alpha_s(\mu_0^2)\frac{1}{2} \right] + \mathcal{O}(\delta^2)) + \cdots . \end{aligned} \tag{37}$$

or either by the n_f-derivative since:

$$\frac{df}{d\beta_0} = \frac{df}{dn_f} \times \frac{d\beta_0}{dn_f}^{-1} \tag{38}$$

Then we can factorize out the Born amplitude Eq.26:

$$\begin{aligned} \left.\frac{d\sigma^{(3)}(\mu_0^2)}{dx_1 dx_2}\right|_{\text{Born}}^{-1} \cdot \frac{d}{d\beta_0}\frac{d^2\sigma^{(3)}(\epsilon,\delta;\mu_0^2)}{dx_1 dx_2} &= \left[-\alpha_s(\mu_0^2)\ \left(\log(\frac{1-\cos\delta}{2}) + 2\,\log{(2-x_1-x_2)} - \frac{13}{3} + \log\frac{q^2}{\mu_0^2} \right.\right. \\ & \left.\left. + \frac{B^S(x_1,x_2)}{2\,B^V(x_1,x_2)} \right) \right] + \mathcal{O}(\delta^2)) + \cdots . \end{aligned}$$

and at the first order approximation the PMC/BLM scale can be fixed numerically imposing:

$$\left[\left.\frac{d\sigma^{(3)}(\mu^2)}{dx_1 dx_2}\right|_{\text{Born}}^{-1} \cdot \left. \left(\frac{d}{dn_f}\frac{d^2\sigma^{(3)}(\epsilon,\delta;\,\mu^2)}{dx_1 dx_2} \right)\right|_{n_f=0} \right]\Bigg|_{\mu^2=\mu^2_{PMC}} = 0 \tag{39}$$

This numerical procedure can be also iterated to the higher orders in α_s, by keeping track of the n_f-terms, leading us to an improvement of the accuracy of the PMC/BLM scale μ^2_{PMC}. Following this procedure we can include all the non-conformal β terms into the running coupling constant for every physical process, setting the renormalization scale at the PMC/BLM scale without necessarily knowing the PMC/BLM analytic form. Thus we end up with a cross section which is formally equal to the corresponding conformal expansion with $\beta = 0$. In this particular case the PMC/BLM scale has the form:

$$\mu^2_{PMC} \simeq q^2 \, (2 - x_1 - x_2)^2 \, \frac{\delta^2}{4} \, e^{-\frac{13}{3} + \frac{B_S(x_1,x_2)}{2\, B_V(x_1,x_2)}}. \tag{40}$$

In this case the coefficient depends on the parton energies x_1, x_2, on the angle parameter δ, and on the scale ratio q^2/μ_0^2 (all these quantities can be written in the form of Lorentz invariants). The different contributions to the coefficient can be also identified, term by term, by considering the most differential cross section (i.e. for the 3-jet case the triple differential cross section), by performing the derivative (or logarithmic derivative) with respect to the corresponding invariant, and then isolating the constant term. This procedure will be discussed in detail in the next section.

V. THE PMC/BLM SCALE AS A FUNCTION OF THE JET MASS RESOLUTION PARAMETER

As shown by Kramer and Lampe [16], one can define a QCD jet by defining a resolution parameter ys as its maximal virtuality. The jet then consists of particles with total invariant mass squared smaller than ys. Using this definition, we will perform the integration of the entire differential cross section, including real and virtual contributions in order to have a IR safe quantity. This gives a y-dependent integrated formula with β_0 dependent terms which can be absorbed into the argument of the running coupling, according to the PMC/BLM prescription.

The entire differential three-jet cross section [22]:

$$\frac{1}{\overline{\sigma}_0} \frac{d\sigma^{(s)} + d\sigma^3}{dy} = \int_y^{1-2y} dz \int_y^{1-y-z} dx \; T[1-x-z, x, z] \alpha_s(Q^2)(1 - \beta_0 \, \alpha_s(Q^2)(\log[x] + \log[z] - \frac{5}{3}......))$$

$$= \alpha_s(Q^2) \, (T(y) - \beta_0 \, \alpha_s(Q^2) \, (C(y) + ...)) \tag{41}$$

$$\equiv T(y)\alpha_s(Q^2) \, (1 - \beta_0 \, \alpha_s(Q^2) \, 2 \log[\frac{\mu_{BLM}}{\sqrt{s}}]) = T(y)\alpha_s(\mu^2_{BLM}); \tag{42}$$

where: $\overline{\sigma}_0 = \sigma_0 \, C_F \, Q^2 \, / 2\pi \, , s = Q^2 \, , x = y_{13} \, , z = y_{23}$,

$$T[x_1, x_2, x_3] \; = \; \frac{2x_1^2 + x_2^2 + x_3^2 + 2x_1(x_2 + x_3)}{x_1 x_3} \tag{43}$$

and

$$\begin{aligned} T[y] \; = \; & \frac{5}{2} - 6y - \frac{9y^2}{2} + 2\text{Log}\left[-2 + \frac{1}{y}\right] \left(3y + \text{Log}\left[-1 + \frac{1}{y}\right]\right) - 3\text{Log}[1-2y] + 3\text{Log}[y] \\ & -2\text{Li}_2\left[2 + \frac{1}{-1+y}\right] + 2\text{Li}_2\left[-\frac{y}{-1+y}\right]; \end{aligned} \tag{44}$$

$$C[y] \;=\; \frac{1}{12}\Big\{9(-1+3y)(11+5y)+(61+18i\pi)\mathrm{Log}[1-2y]+\mathrm{Log}[1-2y]\Big(2y(-103-36y-3i\pi(2+y))$$
$$+6(-3+2y)\mathrm{Log}[1-y]+3\mathrm{Log}[1-2y]\left(-9+14y+y^2+4\mathrm{Log}[1-y]-4\mathrm{Log}[y]\right)\Big)+$$
$$+12\mathrm{ArcTanh}[1-2y]\Big(2\mathrm{Log}[1-2y]^2+y^2(\mathrm{Log}[1-2y]-\mathrm{Log}[y])\Big)+$$
$$(41+38y)(\mathrm{Log}[1-2y]-\mathrm{Log}[y])-\mathrm{Log}[y]+2((31-18y)y+3i\pi(-1+y)(3+y)$$
$$-3(-8+y)y\mathrm{Log}[1-2y]+3(3-2y)\mathrm{Log}[1-y])\mathrm{Log}[y]+3\Big(9+(-30+y)y-8\mathrm{Log}[1-y]\Big)\mathrm{Log}[y]^2$$
$$+24\mathrm{Log}[y]^3-6(-1+y)(3+y)\mathrm{Li}_2\left[\frac{1-y}{y}\right]+6\Big(-3+2y+y^2+8\mathrm{Log}[y]\Big)\mathrm{Li}_2\left[\frac{y}{1-y}\right]$$
$$+6(-1+y)(3+y)\mathrm{Li}_2\left[\frac{1-y}{1-2y}\right]-6\Big(-3+2y+y^2+8\mathrm{Log}[1-2y]\Big)\mathrm{Li}_2\left[\frac{1-2y}{1-y}\right]$$
$$-48\mathrm{Li}_3\left[\frac{y}{1-y}\right]+48\mathrm{Li}_3\left[\frac{1-2y}{1-y}\right]\Big\} \tag{45}$$

Then in the 3-jet case, the BLM-PMC scale as function of the jet-virtuality y, has the analytic form:

$$\hat{\mu}^2 = \mu^2_{PMC/BLM} = s\,\times\,e^{-\frac{5}{3}+\frac{C(y)}{T(y)}} \tag{46}$$

A plot of the PMC/BLM scale against y, the virtuality resolution of the jet, in $e^+e^- \to q\bar{q}g$ is shown in Fig. 2. The result agrees with the BLM scale calculated by Kramer and Lampe in the $\overline{MS}$ scheme. The PMC/BLM prediction is scheme-independent; the specific value of the renormalization scale is rescaled according to the choice of scheme so that all results are commensurate. The PMC/BLM scale also accurately determines n_f, the effective number of flavors in the β-function. As is clear from the QED analog, the renormalization scale reflects the virtuality of the gluon jet; it thus must vanish when the resolution $y\,s$ vanishes. As noted by Kramer and Lampe [16], the renormalization scales determined by the *ad hoc* PMS and FAC (Fastest Apparent Convergence) [23] procedures have the wrong physical behavior at $y\,s \to 0$, since they become infinite $\mu^2 \to \infty$ as the jet resolution and gluon virtuality vanish.

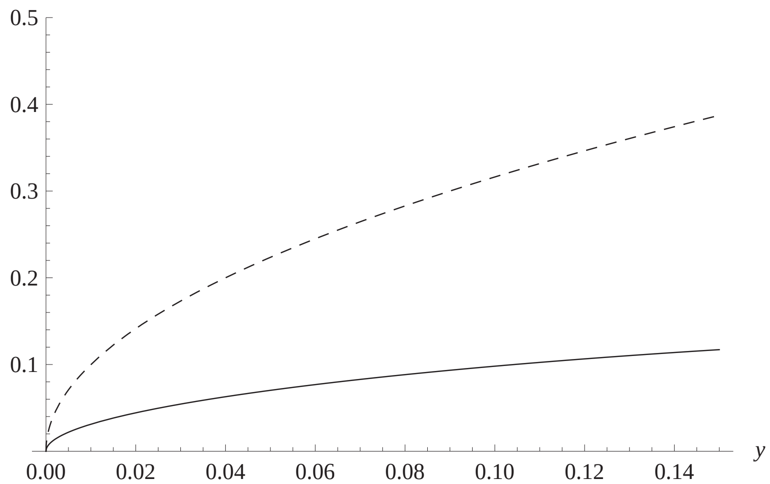

FIG. 2: The PMC/BLM scale, μ_{PMC} (plane line) as a function of the jet resolution parameter y, for $e^+e^- \to q\bar{q}g$. For comparison, $\sqrt{y}$ is also shown (dashed line).

VI. PMC/BLM SCALE FIXING IN THE 3 JET CASE: THE COMPLETE DIFFERENTIAL CROSS SECTION

In the case of the complete differential cross section; i.e., the most differential cross section for a given process without any constrained variables, the PMC/BLM scales depend on the number of flavors n_f and on the independent invariants entering the process. In the case of the three jets we notice that the cross section depends on the color and flavor parameters n_f, N_C, C_F and on the kinematical invariants s_{12}, s_{13}, s_{23} where the label 3 refers to the gluon momentum, and the indices $1, 2$ refer to the quark and anti-quark momenta. On the other hand, the nonconformal terms entering the running coupling depend only on the number of flavors n_f and on a reduced number of kinematical invariants. These terms can be identified by first varying the number of flavors n_f and then the invariant s_{ij}, whereas the constant term can be extracted by simply subtraction at the final step.

Starting with the triple differential cross section for three jets given in Ref.[22]:

$$\frac{d\sigma^{(s)}+d\sigma^{3}}{dz\,dy\,dx} = \tilde{\sigma}_0\,\frac{\alpha_s(Q^2)}{2\pi}\,\delta(1-x-y-z)\Big\{T[z,x,y]\,\Big[1+\frac{\alpha_s(Q^2)}{2\pi}C_F(....)+\frac{\alpha_s(Q^2)}{2\pi}N_C(....)$$

$$-\,\alpha_s(Q^2)\,\beta_0\,\Big(\log[x*y]-\frac{5}{3}\Big)\Big]+\frac{\alpha_s(Q^2)}{2\pi}F[z,y,x]\Big\} \tag{47}$$

with $\tilde{\sigma}_0 = \sigma_0\, C_F s$. For simplicity sake we are using the notation (z, x, y) for respectively the final state gluon-, quark-, antiquark-energy. In order to extract the first order terms related to the $\beta-$ function we can start performing an *ab initio* analysis of the cross section. We can first single out the β_0 coefficient by means of the β_0- derivative, or either by the number of flavors n_f-derivative, using Eq. 38 and then we can factorize out the Born amplitude:

$$\left.\frac{d\sigma^3(Q^2)}{dz\,dy\,dx}\right|_{Born}^{-1}\frac{1}{\alpha_s(Q^2)}\frac{d}{d\beta_0}\,\left(\frac{d\sigma^{(s)}+d\sigma^3}{dz\,dy\,dx}\right) = \left[\log[x\,y]-\frac{5}{3}\right]+O(\alpha_s), \tag{48}$$

$$\left.\frac{d\sigma^3(Q^2)}{dz\,dy\,dx}\right|_{Born} = \tilde{\sigma}_0\,\frac{\alpha_s(Q^2)}{2\pi}\,T[z,x,y]\;\delta(1-x-y-z).$$

Finally, we can extract the weight for each invariant by taking the logarithmic derivative:

$$\omega_i = \frac{d}{d\log(x_i)}\,\left(\left.\frac{d\sigma^3(Q^2)}{dz\,dy\,dx}\right|_{Born}^{-1}\,\frac{1}{\alpha_s(Q^2)}\,\frac{d}{d\beta_0}\,\left(\frac{d\sigma^{(s)}+d\sigma^3}{dz\,dy\,dx}\right)\right) \tag{49}$$

where $x_i = (x, y, z)$. The constant term can be identified by subtracting out all the logarithm terms from the β_0 coefficient. Then at first order approximation in the coupling constant, the μ_{PMC}-scale for the 3-jet differential cross section has the analytic form:

$$\mu^2_{PMC} \simeq Q^2 \times C \times \prod_i x_i^{\omega_i} = Q^2\;x\;y\;e^{-\frac{5}{3}}. \tag{50}$$

A. Commensurate Scale Relations

Relations between observables must be independent of the choice of scale and renormalization scheme. Such relations, called "Commensurate Scale Relations"(CSR) [24–26] are thus fundamental tests of theory, devoid of theoretical conventions. One can compute each observable in any convenient renormalization scheme, such as the $\overline{MS}$ scheme using dimensional regularization. However, the relation between the observables cannot depend on this choice - this is the transitivity property of the renormalization group [3, 7–9]. For example, the PMC relates the effective charge $\alpha_{g_1}(Q^2)$, determined by measurements of the Bjorken sum rule, to the effective charge $\alpha_R(s)$, measured in the total e^+e^- annihilation cross section: $[1-\alpha_{g_1}(Q^2)/\pi]\times[1+\alpha_R(s^*)/\pi] = 1$. The ratio of PMC scales $\sqrt{s}^*/Q \simeq 0.52$ is set by physics; it guarantees that each observable goes through each quark flavor threshold simultaneously as Q^2 and s are raised. Because all $\beta \neq 0$ nonconformal terms are absorbed into the running couplings using PMC, one recovers the conformal prediction [25]; in this case, it is the Crewther relation [27, 28]. Thus by applying the PMC, the conformal commensurate scale relations between observables, such as the Crewther relation, become valid for non-conformal QCD at leading twist.

VII. CONCLUSIONS

As we have shown, the principle of maximal conformality (PMC) provide a consistent method for setting the optimal renormalization scale in pQCD. One shifts the scale so that the β terms in the perturbative series are absorbed into the running coupling. In many cases this can be accomplished simply by absorbing the terms in n_F which arise from coupling constant renormalization. The resulting series is identical to that of the corresponding conformal theory with $\beta = 0$ as given by the Banks-Zaks method. The scale-fixed predictions using the PMC are independent of the choice of renormalization scheme – a key requirement of renormalization group invariance. The results avoid renormalon resummation and agree with QED scale-setting in the Abelian limit. The PMC is the theoretical principle underlying the BLM procedure, commensurate scale relations between observables, and the scale-setting method used in lattice gauge theory [29]. Besides it has been recently shown that for certain observables in 2-jet production the results of the MOM-BLM method are very similar to those of MSYM theory [30][31][32]. The number of active flavors n_f in the QCD β function is also correctly determined.

We have discussed specific methods for efficiently determining either the PMC/BLM renormalization scale analytic form or its numerical value in QCD processes. The analytic form can be determined by varying the subprocess amplitude with respect to each invariant, thus determining the coefficients f_{ij} of $\log p_{ij}^2/\mu_0^2$ in the nonconformal terms in the amplitude. This result can be used to fix individual scales for the contributing skeleton graphs. A single PMC global scale is then determined at NLO by appropriate weighting. On the other hand the numerical value of the PMC scale can be determined also without necessarily knowing the PMC-analytic form, by means of the n_f-derivative of the whole cross section. The two methods completely agree and give rise to the same results.

The global PMC renormalization scale is particularly useful for very complex processes; one only requires the dependence of the calculated subprocess amplitudes on the initial renormalization scale μ_0^2 and n_F, the number of quark flavors appearing from quark loops associated with renormalization. The single global PMC scale, valid at leading order, can thus be derived from basic properties of the perturbative QCD cross section.

Clearly, the elimination of the renormalization scheme ambiguity using the PMC will greatly increase the precision of QCD tests and will also increase the sensitivity of measurements at the LHC and Tevatron to new physics beyond the Standard Model.

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