A novel and self-consistency analysis of the QCD running coupling $\alpha_s(Q)$ in both the perturbative and nonperturbative domains

Qing Yu$^{1,2}$, Xing-Gang Wu$^{1,3}$, Hua Zhou$^{1,2}$, Xu-Dong Huang$^5$, and Jian-Ming Shen$^4$

$^1$ Department of Physics, Chongqing University, Chongqing 401331, People’s Republic of China
$^2$ Department of Physics, Norwegian University of Science and Technology, Høgskoleringen 5, N-7491 Trondheim, Norway
$^3$ Chongqing Key Laboratory for Strongly Coupled Physics, Chongqing 401331, People’s Republic of China and
$^4$ School of Physics and Electronics, Hunan University, Changsha 410082, P.R. China

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The QCD coupling $\alpha_s$ is the most important parameter for understanding the strong interactions among quarks and gluons. By using the well measured effective coupling $\alpha_s^0(Q)$ defined from the Bjorken sum rules as an explicit example, we suggest a novel way to fix the $\alpha_s$ at all scales: The QCD light-front holographic model is adopted for the $\alpha_s$ infrared behavior, and the fixed-order pQCD prediction under the principle of maximum conformality (PMC) is used for the high-energy scale behavior. By applying the PMC, a precise renormalization scheme-and-scale independent perturbative series can be achieved. By further using the physical V-scheme, we observe that a self-consistent and precise $\alpha_s$ running behavior in both the perturbative and the nonperturbative domains with a smooth transition from small to large scales can be achieved.

The QCD running coupling ($\alpha_s$) sets the strength of the interactions of quarks and gluons. The correct and exact $\alpha_s$ value is important for achieving precise QCD predictions, and it is important to find a proper way to fix the $\alpha_s$ value at all scales. On the one hand, in large scale (or short-distance) region, due to the property of asymptotic freedom [1, 2], the magnitude of $\alpha_s$ becomes small and its scale-running behavior is controlled by the renormalization group equation (RGE). Then one can fix its value at large scale by using the measurement of a high-energy observable that can fix the $\alpha_s$-value at a given scale. On the other hand, in small scale (or long-distance) region, a natural extension of $\alpha_s$-behavior derived from the RGE shall meet the unphysical Landau singularity. Various theories and low-energy models have been suggested to set the $\alpha_s$ infrared behavior, cf. the reviews [3, 4]. For example, the dilaton soft-wall modification of the AdS$_5$ metric $e^{4\kappa z^2}$ together with the QCD light-front holography (LFH) [5], where $\kappa$ is a universal confinement scale derived from hadron masses, predicts that $\alpha_s/\pi \to 1$ for $Q^2 \to 0$.

It has been suggested that one can define an effective QCD running coupling at all scales via a perturbatively calculable physical observable [6, 7]. For example, by using the JLAB data on the Bjorken sum rules (BSR) $\Gamma_{1}^{p-n}(Q)$ [8, 9], one can define an effective coupling $\alpha_s^{\gamma_1}(Q)$ via the following way [10–13],

$$\Gamma_1^{p-n}(Q) = \int_0^1 dx (g_1^p(x) - g_1^n(x)) = \frac{g_A}{6}[1 - \alpha_s^{\gamma_1}(Q)],$$

where $\alpha_s^{\gamma_1}(Q) = \alpha_s^0(Q)/\pi$ for simplicity, and $Q$ is the energy scale at which it is measured. $g_1^{p,n}(x)$ are spin structure functions for the proton and neutron with Bjorken scaling variable $x$, and $g_A$ is the nucleon axial charge.

The $\alpha_s^{\gamma_1}(Q)$ implicitly absorbs both the non-perturbative contributions and the higher-order perturbative contributions into the definition. It thus provides a good platform for testing or fixing the running behavior of $\alpha_s$ at all scales, as is the purpose of the present letter.

At high momentum transfer, the effective coupling $\alpha_s^{\gamma_i}$ satisfies asymptotic freedom and it can be expanded as a perturbative series over the $\overline{\text{MS}}$-running coupling $\alpha_s^{\overline{\text{MS}}}$, i.e.

$$\alpha_s^{\gamma_i}(Q) = \sum_{i=1}^{n} r_i^{\overline{\text{MS}}}(Q, \mu_r) a_s^{\overline{\text{MS}},i}(\mu_r),$$

where $\mu_r$ is the renormalization scale and the perturbative coefficients $r_i$ have been calculated up to four-loop QCD corrections [14, 15]. Using this higher-loop pQCD series, we can achieve a precise prediction on $\alpha_s^{\gamma_i}(Q)$ at the high momentum transfer, and by requiring its value and its slope be matched to a low-energy model such as [16] 1

$$a_s^{\gamma_i,\text{LFH}}(Q) = e^{-Q^2/4\kappa^2},$$

some attempts have been done to fix an interface scale and a smooth connection between perturbative and non-perturbative hadron dynamics, cf. Refs.[16–19].

Previously, the scheme-and-scale dependent fixed-order pQCD series (2) has been directly adopted to do the matching [16–18], whose renormalization scale is set as the guessed typical momentum transfer of the process (e.g. $Q$) and where an arbitrary range $[Q/2, 2Q]$ is assigned to estimate the scale uncertainty. Due to the mismatching of $\alpha_s$ and the coefficients at each perturbative

1 We adopt this model, since its prediction agrees with the hadronic data extracted from various observables as well as the predictions of various models with the built-in confinement and lattice simulations.
order, this uncertainty is unavoidable, whose magnitude depends heavily on the how many terms of the pQCD series are known and the convergence of the pQCD series, and it is then conventionally treated as an important systematic error of the pQCD prediction. Numerically, it has been found that the scale errors are still sizable in intermediate and low-energy region even for the four-loop series due to larger $\alpha_s$ in those regions. This mainly input and unwanted scale error thus greatly affects the accuracy of the matching. Thus it is important to adopt a proper scale-setting approach so as to achieve a more accurate fixed-order prediction.

In the literature, the principle of maximum conformality (PMC) [20–24] has been suggested to eliminate the ambiguities caused by the use of the guessed scale. The PMC recursively uses the RGE and fixes the correct magnitude of $\alpha_s$ by absorbing all the $\{\beta_i\}$-related non-conformal terms via a systematic way, while remaining the scale-independent conformal coefficients. This leads to a scheme and scale invariant pQCD prediction [25], which agrees with the standard renormalization group invariance (RGI) [26–31]. Many successful applications of the PMC can be found in the reviews [32, 33].

In year 2017, the PMC multi-scale approach has been applied to do the matching of $a_s^{\alpha_s}(Q)$ in both the perturbative and nonperturbative domains [19], in which distinct PMC scales at each order in the perturbative domain are determined so as to absorb different categories of $\{\beta_i\}$-terms into the corresponding $\alpha_s$. The authors found that a significantly more precise matching of $a_s^{\alpha_s}(Q)$ can indeed be achieved due to the elimination of renormalization scale ambiguity, but they also found a “self-consistency problem”, i.e. the PMC scales at certain orders in the $\overline{\text{MS}}$-scheme are smaller than the determined scale $Q_0$ which represents the transition between the perturbative and non-perturbative domains of QCD. This will affects the precision of the pQCD prediction. In this letter, as a new attempt, we show that the “self-consistency problem” mentioned in Ref.[19] can be solved by applying the newly suggested PMC all-orders single-scale approach [34, 35] together with the using of the physical $V$-scheme [36–39].

The PMC single-scale approach determines a single effective PMC scale by using the RGE, which represents the overall effective momentum flow of the process and replaces all the multi-scales at each order on the basis of a mean value theorem. The PMC single-scale approach is a reliable substitution for the PMC multi-scale approach, which can further greatly suppress the residual scale dependence due to unknown perturbative terms [40]. The PMC predictions are scheme independent, which are ensured by the PMC conformal series, and by using the commensurate scale relations among different schemes [41], the determined PMC scale may be larger than the critical scale $Q_0$ by choosing a proper scheme other than the $\overline{\text{MS}}$-scheme, then a solution of “self-consistency problem” can be achieved. We have tried various intermediate schemes and found that the $V$-scheme is the best one. The gauge-independent $V$-scheme has some advantages. It corrects the static potential by higher-order QCD corrections, and it is particularly well-suited to summing the effects of gluon exchange at low momentum transfer, such as in evaluating the final-state interaction corrections to heavy quark production [42], or in evaluating the hard-scattering matrix elements underlying exclusive processes [43]. And different from the $\overline{\text{MS}}$-scheme, the physical $V$-scheme also models a smooth transition of the QCD running coupling through the thresholds of heavy quark productions, since it corrects the massive dependent corrections in running effect of the QCD coupling constant [44].

For the purpose, we transform the known four-loop $\overline{\text{MS}}$-scheme series (2) of $a_s^{\alpha_s}$ into the $V$-scheme one,

$$a_s^{\alpha_s}(Q) = r_{1,0}^V a_s^V(\mu_r) + (r_{2,0}^V + \beta_0^V a_s^V) a_s^{\alpha_s}(\mu_r) + (r_{3,0}^V + \beta_1^V a_s^V) a_s^{\alpha_s}(\mu_r) + (r_{4,0}^V + \beta_2^V a_s^V) a_s^{\alpha_s}(\mu_r) + \sum_{i,j} r_{i,j}^V,$$

where the QCD degeneracy relations [45] have been implicitly used to transform $\overline{\text{MS}}$ into $V$ and the $V$-scheme $\{\beta_i^V\}$-functions can be derived by using their relations to the $\overline{\text{MS}}$-scheme ones, which are known up to five-loop level [46–48], $\beta_i^V(a_s^V) = (\partial a_s^V/\partial a_s^\overline{\text{MS}}) \beta_i^\overline{\text{MS}}(a_s^\overline{\text{MS}})$. $r_{i,j}^V$ ($j \neq 0$) are general functions of $\ln(\mu_r^2/Q^2)$; i.e.

$$r_{i,j}^V = \sum_{k=0}^j C_k^j \ln^k(\mu_r^2/Q^2) r_{i-k,j-k}^V,$$  

where the combination coefficients $C_k^j = j!/k!(j-k)!$ and the coefficients $r_{i,j}^V|_{\mu_r=q}$. The magnitude of $\alpha_s$ can be determined by using the $\{\beta_i^V\}$-functions. Following the standard PMC procedures, by requiring all the RGE-involved $\{\beta_i\}$-terms to zero, one can determine a scale-invariant optimal scale $Q_s^V$ of the process and obtain a conform series as follows

$$a_s^{\alpha_s}(Q_s)|_{\text{PMC}} = \sum_{i=1}^4 r_{i,0}^V a_s^{\alpha_s,V,i}(Q_s),$$

where the PMC scale $Q_s$ is a function of $Q$, which by using the four-loop pQCD series, can be fixed up to next-to-next-to-leading-log (NNLL) accuracy,

$$\ln \frac{Q_s^2}{Q^2} = T_0 + T_1 a_s^V(Q) + T_2 a_s^{\alpha_s^2}(Q),$$

where

$$T_0 = -\frac{r_{1,0}^V}{r_{1,1}^V}. \quad (8)$$
T_1 = \frac{2(\hat{r}_{2,0}^Y r_{2,1}^Y - \hat{r}_{1,0}^Y r_{1,0}^Y)}{r_{1,0}^Y} + \frac{(\hat{r}_{2,1}^Y - \hat{r}_{1,0}^Y)}{r_{1,0}^Y} \beta_0, \quad (9)
\begin{align*}
T_2 &= \frac{4(\hat{r}_{1,0}^Y r_{2,0}^Y r_{3,1}^Y - \hat{r}_{2,0}^Y r_{2,2}^Y)}{r_{1,0}^Y r_{1,0}^Y} + 3(\hat{r}_{1,0}^Y r_{2,1}^Y r_{3,0}^Y - \hat{r}_{1,0}^Y r_{1,0}^Y) \\
&= \frac{3(\hat{r}_{2,1}^Y - \hat{r}_{1,0}^Y)}{2r_{1,0}^Y r_{1,0}^Y} \beta_1 + \frac{\hat{r}_{2,0}^Y}{r_{1,0}^Y} + \frac{3\hat{r}_{1,0}^Y}{r_{1,0}^Y} \beta_0 \\
&= \frac{(2\hat{r}_{1,0}^Y r_{2,2}^Y - 2\hat{r}_{1,0}^Y r_{2,1}^Y r_{3,1}^Y - \hat{r}_{1,0}^Y r_{1,0}^Y)}{r_{1,0}^Y} \beta_0 \\
&= \frac{(2\hat{r}_{1,0}^Y r_{2,2}^Y - 2\hat{r}_{1,0}^Y r_{2,1}^Y r_{3,1}^Y + \hat{r}_{1,0}^Y r_{1,0}^Y)}{r_{1,0}^Y} \beta_0 \\
&= \frac{(2\hat{r}_{1,0}^Y r_{2,2}^Y - 2\hat{r}_{1,0}^Y r_{2,1}^Y r_{3,1}^Y)}{r_{1,0}^Y} \beta_0. \quad (10)
\end{align*}

It is noted that the perturbative series of \(a_s^{q_1}(Q)|_{\text{PMC}}\) is explicitly free of \(\mu_r\), leading to a precise scheme-and-scale invariant fixed-order prediction. And due to the elimination of divergent renormalon terms, the convergence of the pQCD series is greatly improved.

![FIG. 1. The calculated effective scale \(Q_\star\) up to NNLL accuracy under \(\overline{\text{MS}}\) scheme and V scheme, respectively.](image)

To do the numerical calculation, we adopt \(a_s^{\overline{\text{MS}}}(M_Z) = 0.1179 \pm 0.0010\) [49] to fix the QCD asymptotic scale \(\Lambda\), and we obtain \(\Lambda^{\overline{\text{MS}}} = 0.343 \pm 0.015\) GeV and \(\Lambda^Y = 0.438 \pm 0.019\) GeV for three active flavors. As a typical example, the perturbative series (6) for \(n_f = 3\) becomes

\[a_s^{q_1}(Q)|_{\text{PMC}} = a_s^Y(Q_\star) + 3.15a_s^{Y,2}(Q_\star) + 24.06a_s^{Y,3}(Q_\star) + 51.36a_s^{Y,4}(Q_\star),\]

where \(Q_\star\) satisfies

\[\ln \frac{Q_\star^2}{Q^2} = 0.58 + 2.06a_s^Y(Q) - 7.41a_s^{Y,2}(Q),\]  

which leads to \(Q_\star = 3.98\) GeV for \(Q = 3\) GeV. Fig. 1 shows how \(Q_\star\) changes with \(Q\), where \(Q_\star\) under \(\overline{\text{MS}}\)-scheme is also presented as a comparison. Fig. 1 shows that \(Q_\star\) under V-scheme has a faster increase with the increment of \(Q\) than the case of \(\overline{\text{MS}}\)-scheme. Thus the previous puzzle of \(Q_\star < Q_0\) could be avoided. Because

\[\ln Q^2/Q^2\] is a perturbative series, its unknown perturbative terms shall lead to the first kind of residual scale dependence [50], and as a conservative estimation, its magnitude could be estimated by taking the unknown term as \(\pm 7.41a_s^{Y,2}(Q)\), which gives \(\Delta Q_\star \simeq (0.31 \pm 0.13)\) GeV for \(Q = 3\) GeV. Lately, we observe such scale uncertainty shall be further constrained by the matching of \(a_s^{q_1}(Q)\) in perturbative and non-perturbative domains.

Similarly, the unknown higher-order terms of Eq.(11) shall lead to the second kind of residual scale dependence [51], which can be estimated by using a more strict Padé approximation approach (PAA) due to more loop terms have been known [52]. The PAA offers a feasible conjecture that yields the \(5_{\text{th}}\)-order terms from the given \(4_{\text{th}}\)-order perturbative series, and a \([N/M]\)-type approximant \(\rho_M(Q)|_{\text{PMC}}\) is defined as

\[\rho_M^{[N/M]}(Q) = a_s^Y(Q_\star) + b_0a_s^Y(Q_\star) + \cdots + b_Na_s^{Y,2}(Q_\star) + 1 + c_1a_s^Y(Q_\star) + \cdots + c_Ma_s^{Y,3}(Q_\star),\]

where the parameter \(M \geq 1\) and \(N + M = 3\). The known coefficients \(\hat{r}_{i,0}^Y\) determine the parameters \(b_i \in [0, N]\) and \(c_j \in [1, M]\), which inversely predicts a reasonable value for the uncalculated \(N^2\)LO-coefficient \(\hat{r}_{5,0}^Y\) [53], i.e.

\[\hat{r}_{5,0}^{\text{PAA}}(Q_\star) = \hat{r}_{5,0}^Y a_s^{Y,5}(Q_\star) + \cdots,\]  

Then the uncertainty from the unknown terms could be estimated by \(\pm \hat{r}_{5,0}^{\text{PAA}} a_s^{Y,5}(Q_\star) = \pm 232.22a_s^{Y,5}(Q_\star)\).

It is found that the LFH model \(a_s^{q_1,\text{LFH}}(Q)\) can be naturally matched to the conformal perturbative series, since it is consistent with the conformal behavior at \(Q^2 \rightarrow 0\). To do the matching, we require the magnitudes and the derivatives of both the LFH \(a_s^{q_1,\text{LFH}}(Q)\) and the prediction \(a_s^{q_1}(Q)|_{\text{PMC}}\) to be the same at the critical scale \(Q_0\).

We present the matching of \(a_s^{q_1,\text{LFH}}(Q)\) and \(a_s^{q_1}(Q)|_{\text{PMC}}\) under the V-scheme up to \(N^3\)LO-order QCD corrections in Fig. 2, where the available data which are for low- and intermediate-energy region issued by various experimental groups [10, 54–63] have also been presented. The determined critical scale \(Q_0 = 1.51^{+0.16}_{-0.31}\) GeV, whose errors are caused by the first kind of residual scale dependence and the second kind of residual scale dependence together with the error of \(\Delta a_s(M_Z) = \pm 0.0010\). The input parameter of the LFH model \(\kappa = 0.64^{+0.07}_{-0.14}\) GeV [3], and the PMC scale \(Q_\star(Q_0) \simeq 1.58^{+0.09}_{-0.01}\) GeV. We observe

\[2\] By using the PAA, the predicted \(\Delta Q_\star\) is similar which shall also be constrained by the matching and get the close error range.

\[3\] This value is slightly larger than \(\sim 1/2\) GeV, which incorporates high-twist contributions, since the high twist terms could have sizable contributions to \(\Gamma^{\text{LE}}_{\text{in}}(Q)\) in low-energy region [64].
FIG. 2. The matching of the LFH low-energy $a_{g_{1}}^{\text{LH}}(Q)$ and the PMC prediction of $a_{g_{1}}^{\text{PMC}}(Q)$ under the $V$-scheme up to the N$^3$LO-order QCD corrections. The shaded band is the uncertainty caused by squared averages of the residual scale dependence due to the uncalculated higher-order terms and $\Delta\alpha_s(\overline{\text{MS}})(M_Z) = \pm 0.0010$.

that $Q_*(Q_0) > Q_0$, thus the previous “self-consistency problem” is solved by using the $V$-scheme and the PMC single-scale approach. Moreover, the quality of fit for the matched $a_{g_{1}}^{\text{PMC}}$ can be measured by using the parameter $\chi^2/d.o.f$ [49], which represents the quality $\chi^2$ over the number of experiment data points $N$ and is defined as

$$\chi^2/d.o.f = \frac{1}{N - d} \sum_{j=1}^{N} \left[ \frac{1}{\sigma_{j,\text{stat}}^2 + \sigma_{j,\text{the.}}^2} \right] \left[ a_{g_{1}}^{\text{PMC},\text{exp.}}(Q_j) - a_{g_{1}}^{\text{PMC},\text{the.}}(Q_j) \right]^2$$

where $\sigma_{j,\text{stat}}$ stands for the statistical error at each data point $Q_j$, “the.” stands for theoretical prediction and “exp.” stands for the experimental value. We adopt $N = 70$, which are given in Refs. [10, 54–63], and $d = 2$ due to two input parameters ($\kappa$ and $Q_0$). Our numerical calculation shows $\chi^2/d.o.f \simeq 0.18$, which corresponds to $p \simeq 99\%$, indicating a good goodness-of-fit and the reasonableness of the fitted input parameters.

As a final remark, we also calculate the correlation coefficient $\rho_{XY}$ [49] to show to what degree the matched $\alpha_s^{\text{PMC}}$ are correlated to the 70 data points

$$\rho_{XY} = \frac{\text{Cov}(X, Y)}{\sigma_X \sigma_Y},$$

where $X$ and $Y$ stand for the experimental data on $\alpha_s^{\text{exp.}}$ and the theoretically predicted ones, respectively. The covariance $\text{Cov}(X, Y) = E[(X - E(X))(Y - E(Y))] = E(XY) - E(X)E(Y)$, where $E(X)$ stands the expectation value of $X$, $\sigma_{X,Y}$ is the standard deviations of $X$ or $Y$. Numerically, we obtain $\rho_{XY} \sim 0.96 \pm 0.02$, which indicates a high consistency between the predicted $\alpha_s^{\text{PMC}}$ and the measured one.

**Summary.** The QCD running coupling is one of the most important parameters for QCD theory. In this letter, by using the effective coupling $a_{s}^{\text{eff}}(Q)$ as an explicit example, we have shown that a self-consistency QCD running coupling $\alpha_s(Q)$ in both the perturbative and non-perturbative domains can be achieved by applying the PMC singlet-scale approach. Though the PMC prediction is scheme independent, a proper choice of scheme could have some subtle differences. Fig. 1 shows that the effective PMC scale $Q_*$ under the $V$-scheme has a faster increase with the increment of $Q$ than the case of MS-scheme. Thus the previous puzzle of $Q_* < Q_0$ is eliminated. The PMC eliminates the conventional renormalization scale ambiguity, and its single-scale setting approach greatly depresses the residual scale dependence due to uncalculated perturbative terms, thus a more accurate fixed-order pQCD prediction can be achieved. We observe that the LFH low-energy model $a_{g_{1}}^{\text{LH}}(Q)$ can be naturally matched to the PMC conformal perturbative series $a_{g_{1}}^{\text{PMC}}(Q)$ over the physical $V$-scheme, and as shown by Fig. 2, one can achieve a reasonable and smooth connection between the perturbative and non-perturbative domains.

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* yuq@cqu.edu.cn
† wuxg@cqu.edu.cn
‡ zhouhua@cqu.edu.cn
§ hxud@cqu.edu.cn
* shenjm@hnu.edu.cn
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