Static QCD Potential at Three-Loop Order

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We compute the purely gluonic contribution to the static QCD potential at three-loop order. This completes computation of the static potential at this order.

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For more than 30 years, the static QCD potential $V_{\rm QCD}(r)$ has been studied extensively for the purpose of elucidating the nature of the interaction between a heavy quark and antiquark. Generally, $V_{\rm QCD}(r)$ at short distances can be computed accurately by perturbative QCD. On the other hand, the potential shape at long distances should be determined by nonperturbative methods, such as lattice simulations or phenomenological potential-model analyses or computations based on string-inspired models.

Computations of $V_{\rm QCD}(r)$ in perturbative QCD have a long history. At the tree level, $V_{\rm QCD}(r)$ is merely a Coulomb potential, $-C_F\alpha_S/r$ ($C_F = 4/3$ is a color factor), arising from a one-gluon-exchange diagram. The one-loop corrections (with massless and/or massive internal quarks) were computed in [1,2]. The two-loop correction (with massless internal quarks) was computed in [3]. The two-loop correction due to massive internal quarks was computed in [4] (partly corrected in [5]) [6]. The logarithmic correction at three loop originating from the ultrasoft scale was first pointed out in [1] and computed in [8]. Renormalization-group (RG) improvement of $V_{\rm QCD}(r)$ at next-to-next-to-leading logarithmic order was performed in [9]. A logarithmic contribution at $\mathcal{O}(\alpha_S^5)$ was computed in [10]. The contributions of the massless quark loops to the three-loop correction were computed in [11]. The only remaining correction at three-loop order is the purely gluonic contribution, which we compute in this Letter.

For a long time, the perturbative QCD predictions of $V_{\rm QCD}(r)$ were *not* successful in the intermediate distance region, relevant to the bottomonium and charmonium states. In fact, the perturbative series turned out to be poorly convergent at $r \gtrsim 0.1$ fm; uncertainty of the series is so large that one could hardly obtain meaningful predictions in this distance region. Even if one tries to improve the perturbation series by certain resummation prescriptions (such as RG improvement), scheme dependence of the results turns out to be very large; hence, one cannot obtain accurate predictions of the potential in this region. It was later pointed out that the large uncertainty of the perturbative prediction can be understood as caused by the $\mathcal{O}(\Lambda_{\rm QCD})$ infrared (IR) renormalon contained in $V_{\rm QCD}(r)$ [12].

The situation has changed dramatically since the discovery of the cancellation of $\mathcal{O}(\Lambda_{\rm QCD})$ renormalons in the total energy of a static quark-antiquark pair $E_{\rm tot}(r) \equiv V_{\rm QCD}(r) + 2m_{\rm pole}$ [13]. Convergence of the perturbative series for $E_{\rm tot}(r)$ improved drastically, and much more accurate perturbative predictions for the potential shape became available. It was understood that a large uncertainty originating from the $\mathcal{O}(\Lambda_{\rm QCD})$ renormalon in $V_{\rm QCD}(r)$ can be absorbed into twice the quark pole mass $2m_{\rm pole}$. Once this is achieved, perturbative uncertainty of $E_{\rm tot}(r)$ is estimated to be much smaller.

Then it was readily recognized that perturbative convergence of $V_{\rm QCD}(r)$ can be improved by adding a (r-independent) constant at each order of the perturbative expansion, since the $\mathcal{O}(\Lambda_{\rm QCD})$ renormalon is r independent. The conventional prescription to fix $V_{\rm QCD}(r) \to 0$ at $r \to \infty$ is not optimal as the convergence of the perturbative series is worse at larger r; rather, it is better to fix $V_{\rm QCD}(r)$ at some small distance. As it turned out, $V_{\rm QCD}(r)$ becomes steeper at $r \gtrsim 0.1$ fm as the order of the expansion is raised; hence, the convergence of the perturbative series becomes worse if we fix $V_{\rm QCD}(r)$ at $r \to \infty$. This feature, that the perturbative potential becomes steeper than the Coulomb potential as r increases, is understood, within perturbative QCD, as an effect of the *running* of the strong coupling constant [14]. In fact, several studies have shown that perturbative predictions for $V_{\rm QCD}(r)$ agree well with phenomenological potentials and lattice calculations of $V_{\rm QCD}(r)$ in the intermediate distance region [5,14–16].

The improvement of the situation opened up vast applications of the QCD potential in heavy quarkonium physics [17]. For instance, higher-order computations of $V_{\rm QCD}(r)$ play crucial roles in precise determinations of m_c, m_b, m_t from the masses of charmonium, bottomonium, and (would-be) toponium states. The three-loop correction to $V_{\rm QCD}(r)$ is one of the missing parts in these computations and also in recent efforts to complete next-to-next-to-next-to-leading order corrections to heavy quark production near threshold at e^+e^- colliders [18]. Another application is a precise determination of α_S, from comparison of the perturbative prediction and lattice computations of $V_{\rm QCD}(r)$ [19].

The static QCD potential is defined from an expectation value of the Wilson loop as

$$V_{\rm QCD}(r) = -\lim_{T\to\infty}\frac{1}{iT}\log\frac{\langle 0|{\rm Tr}Pe^{ig\oint_C dx^\mu A_\mu}|0\rangle}{\langle 0|{\rm Tr}\mathbf{1}|0\rangle} = \left(\frac{\mu^2 e^{\gamma_E}}{4\pi}\right)^\epsilon \int\frac{d^d\vec{q}}{(2\pi)^d}e^{i\vec{q}\cdot\vec{r}}\left[-4\pi C_F\frac{\alpha_V(q)}{q^2}\right], \quad (1)$$

where $q = |\vec{q}|$ and C is a rectangular loop of spatial extent r and time extent T. The second equality defines the V-scheme coupling constant, $\alpha_V(q)$, in momentum space. We employ dimensional regularization with one temporal dimension and $d = D - 1 = 3 - 2\epsilon$ spatial dimensions. A prefactor is included such that $\alpha_V(q)$ is defined to be dimensionless; $\gamma_E = 0.5772\ldots$ denotes the Euler constant.

In perturbative QCD, $\alpha_V(q)$ is calculable in the series expansion of the strong coupling constant. We denote the perturbative evaluation of $\alpha_V(q)$ as

$$\alpha_V^{\rm PT}(q) = \alpha_S(\mu)\sum_{n=0}^{\infty}P_n(\ell)\left(\frac{\alpha_S(\mu)}{4\pi}\right)^n, \quad (2)$$

with

$$\ell = \log(\mu/q). \quad (3)$$

Here, $\alpha_S(\mu)$ denotes the strong coupling constant renormalized at the renormalization scale μ, defined in the modified minimal subtraction ($\overline{\rm MS}$) scheme, and $P_n(\ell)$ denotes an nth-degree polynomial of ℓ. The RG equation of $\alpha_S(\mu)$ is given by

$$\mu^2\frac{d}{d\mu^2}\alpha_S(\mu) = -\alpha_S(\mu)\sum_{n=-1}^{\infty}\beta_n\left(\frac{\alpha_S(\mu)}{4\pi}\right)^{n+1}, \quad (4)$$

where β_n represents the $(n+1)$-loop coefficient of the beta function [20]. For $n \le 2$, the only part of the polynomial $P_n(\ell)$ that is not determined by the RG equation is $a_n \equiv P_n(0)$. For $n \ge 3$, $P_n(\ell)$ includes IR divergences in terms of poles of ϵ and associated logarithms, whose coefficients are not determined by β_i's. At three-loop order, we have

$$P_3(\ell) = a_3 + (6a_2\beta_0 + 4a_1\beta_1 + 2a_0\beta_2)\ell + (12a_1\beta_0^2 + 10a_0\beta_0\beta_1)\ell^2 + 8a_0\beta_0^3\ell^3, \quad (5)$$

$$a_3 = \bar{a}_3 + \frac{8}{3}\pi^2 C_A^3\left(\frac{1}{\epsilon} + 6\ell\right). \quad (6)$$

$C_F = (N_c^2 - 1)/(2N_c)$ and $C_A = N_c$ denote the eigenvalues of the quadratic Casimir operators for the fundamental and adjoint representations, respectively, of the color $SU(N_c)$ gauge group; $N_c = 3$ in QCD.

The IR divergence is an artifact of the strict perturbative expansion of $V_{\rm QCD}(r)$ in α_S; beyond naive perturbation theory, this IR divergence is absent and regularized by the energy difference between color-singlet and octet intermediate states. The difference between $V_{\rm QCD}(r)$ and its perturbative expansion $[V_{\rm QCD}(r)]_{\rm PT}$ can be treated systematically within the effective field theory "potential nonrelativistic QCD" [21]. ($[V_{\rm QCD}(r)]_{\rm PT}$ is obtained from $V_{\rm QCD}(r)$ if we replace $\alpha_V(q)$ in Eq. (1) by $\alpha_V^{\rm PT}(q)$.) This difference,

$$[V_{\rm QCD}(r)]_{\rm US} = V_{\rm QCD}(r) - [V_{\rm QCD}(r)]_{\rm PT}, \quad (7)$$

is given by contributions of ultrasoft (US) degrees of freedom [22]. In the region $r \ll \Lambda_{\rm QCD}^{-1}$, the leading-order contribution to $[V_{\rm QCD}(r)]_{\rm US}$ in double expansion in α_S and $\log(\alpha_S)$ is readily obtained from the result of [8] as

$$[V_{\rm QCD}(r)]_{\rm US,LO} = \frac{C_F C_A^3\alpha_S^4}{24\pi r}\left[\frac{1}{\epsilon} + 8\log(\mu r) - 2\log(C_A\alpha_S) + \frac{5}{3} + 6\gamma_E\right]. \quad (8)$$

Upon Fourier transform, $1/\epsilon$ and $\log\mu$ terms of Eqs. (6) and (8) cancel each other. In general, at $r < \Lambda_{\rm QCD}^{-1}$, one may perform an operator-product expansion of $[V_{\rm QCD}(r)]_{\rm US}$ as a multipole expansion in r. In this case, nonperturbative contributions to $[V_{\rm QCD}]_{\rm US}$ are parametrized in the form of nonlocal gluon condensates.

We may classify $\bar{a}_3$ in (6) according to the powers of the number of flavors n_l of the internal quarks:

$$\bar{a}_3 = n_l^3\bar{a}_3^{(3)} + n_l^2\bar{a}_3^{(2)} + n_l\bar{a}_3^{(1)} + \bar{a}_3^{(0)}. \quad (9)$$

The purpose of this Letter is to compute $\bar{a}_3^{(0)}$.

Let us describe our calculational procedure. At tree level and at one-loop order, computation of $[V_{\rm QCD}(r)]_{\rm PT}$ is more or less trivial. The two-loop correction to $[V_{\rm QCD}(r)]_{\rm PT}$ is expressed in terms of five master integrals, all of which are expressed in terms of the Γ function and rational functions of ϵ [23]. Hence, we may easily obtain expansion coefficients in ϵ necessary for the three-loop computation.

We first generate three-loop Feynman diagrams for the scattering of static quark and antiquark using GRACE [24] and QGRAF [25]. There are about 20 000 diagrams; we confirmed that the diagrams generated by the two programs coincide. The next step is to eliminate iterations of the lower-order potential at the diagram level, which involves rearrangements of color factors associated with diagrams; we use the general algorithm developed in [26]. This procedure eliminates diagrams that contain pinch singularities. Subsequently, the color factor for each diagram is simplified using the program COLOR provided in [27].

Our computation is carried out in Feynman gauge. The loop integrals are classified according to different numerators and denominators. At an early stage of the computation, we identify those integrals which are trivially zero in dimensional regularization and eliminate them. To reduce the labor of the computation, we collect integrands with a common denominator and cancel terms in the numerator against the denominator as much as possible, by appropriately expressing the numerator by combinations of factors

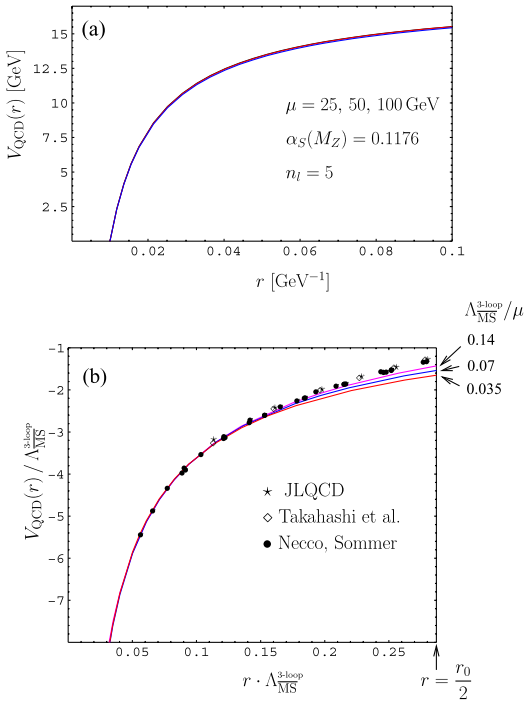

FIG. 1 (color online). $V_{\rm QCD}(r) = [V_{\rm QCD}(r)]_{\rm PT} + [V_{\rm QCD}(r)]_{\rm US}$ up to $\mathcal{O}(\alpha_s^4)$ and $\mathcal{O}(\alpha_s^4 \log\alpha_S)$. (a) In the toponium region, three lines, corresponding to $\mu = 25$, 50, and 100 GeV, are plotted with $n_l = 5$. (b) Comparison with the lattice computations in the quenched approximation [15,30]. We set $n_l = 0$. The distance region corresponds roughly to the size of $\Upsilon(1S)$ state.

in the denominator. After these processes, we were able to express the three-loop correction to $[V_{\rm QCD}(r)]_{\rm PT}$ in terms of about 1700 integrals.

Following the standard procedure of contemporary loop computations, these integrals are expressed in terms of a small set of integrals (master integrals) through the reduction procedure using integration-by-parts (IBP) identities [28]. To carry out the reduction efficiently, we use the LAPORTA algorithm [29]. In addition to known techniques, we implement some improvement to this reduction algorithm. For instance, we temporarily assign a numerical value to D and reduce integrals to simpler ones using IBP identities. The reduction process completes swiftly since manipulation of numerics is considerably faster than symbolic manipulation involving rational functions of D. We retrace the reduction process and identify a minimal set of necessary IBP identities for this reduction. Then we reprocess the reduction (without assigning a numerical value to D) using the minimal set of identities, after rearranging the order of these identities optimally. In the end, the three-loop correction to $[V_{\rm QCD}(r)]_{\rm PT}$ is expressed in terms of 40 master integrals. All the processes are automatized, and the integrals are reduced one after another. The reduction processes required roughly 3 weeks' CPU time of a contemporary desktop computer with 5 GB memory.

Out of 40 master integrals, 17 integrals can be expressed in terms of the Γ function and rational functions of D. The rest of the master integrals are expanded in Laurent series in ϵ, and their expansion coefficients are evaluated analytically if possible and numerically otherwise. (For some expansion coefficients, analytical values are available in the literature.) Numerical evaluation of the expansion coefficients are carried out in two ways: (a) by evaluating Feynman parameter integrals using sector decomposition and (b) by evaluating integrals in Mellin-Barnes representation. The typical relative accuracy in the numerical evaluation of the expansion coefficients is of the order of 10^{-5}. Details of our computation will be described elsewhere.

Our final result reads

$$\bar{a}_3^{(0)} = [502.22(12)]C_A^3 + [-136.8(14)]\frac{d_F^{abcd}d_A^{abcd}}{N_A}, \tag{10}$$

with the color factor $d_F^{abcd}d_A^{abcd}/N_A = N_c(N_c^2+6)/48$ [27]. For completeness, we combine our result with that of [11] and list the numerical values of $\bar{a}_3$, defined in Eq. (6), for $N_c = 3$ and $n_l = 3, 4, 5$ in Table I.

At every stage of the computation we performed numerous cross-checks. At every step we have written (at least) two independent programs and checked that results mutually agree. We derived many relations among different types of integrals and checked that, when the integrals are expressed by master integrals, these relations are satisfied. Renormalizability of $[V_{\rm QCD}(r)]_{\rm PT}$ with the known renormalization constant of the strong coupling constant, as well as reproduction of known IR divergence, provides nontrivial cross-checks. We have reproduced $\bar{a}_3^{(3)}$, $\bar{a}_3^{(2)}$, and the coefficient of C_F^2 in $\bar{a}_3^{(1)}$ [11] analytically. We also computed the coefficients of C_A^2, C_AC_F, and $d_F^{abcd}d_F^{abcd}/N_A$ in $\bar{a}_3^{(1)}$ numerically and confirmed that our results agree with those of [11] within the estimated errors. The last comparison provides a strong cross-check on the correctness and accuracy of our result (10), since the expansion coefficients necessary to compute the result (10) are common to the ones necessary to compute $\bar{a}_3^{(3)}$, $\bar{a}_3^{(2)}$, $\bar{a}_3^{(1)}$, except for two coefficients.

Now we compute $V_{\rm QCD}(r)$, as given by the sum of $[V_{\rm QCD}(r)]_{\rm PT}$ and $[V_{\rm QCD}(r)]_{\rm US}$, including all the corrections up to $\mathcal{O}(\alpha_s^4)$ and $\mathcal{O}(\alpha_s^4 \log\alpha_S)$. Namely, we use the series expansion (2) up to $n = 3$ for the former and Eq. (8) for the latter.

TABLE I. Numerical values of $\bar{a}_3$, defined in Eq. (6), for different values of n_l.

n_l	3	4	5
$\bar{a}_3$	5199(3)	3160(3)	1460(3)

In Fig. 1(a) we plot our prediction for $V_{\rm QCD}(r)$ in the distance region corresponding to (would-be) toponium states. Three lines are plotted, corresponding to $\mu = 25$, 50, and 100 GeV, with $n_l = 5$ and $\alpha_S(M_Z) = 0.1176$. We added a constant to each prediction such that it takes a common value at $r = 0.01\ \mathrm{GeV}^{-1}$. The differences of the three lines are hardly visible, showing stability of the prediction.

In Fig. 1(b) we compare our prediction with the lattice data in the quenched approximation [15,30]. Accordingly we set $n_l = 0$. We used the central value of $r_0\Lambda^{\rm 3\text{-}loop}_{\overline{\rm MS}} = 0.574 \pm 0.042$ [19] to fix the relation between the lattice scale and $\Lambda^{\rm 3\text{-}loop}_{\overline{\rm MS}}$, where r_0 denotes the Sommer scale. Hence, the only adjustable parameters in our comparison are r-independent constants to be added to the potentials, whose values are chosen such that all the potentials coincide at $r\Lambda^{\rm 3\text{-}loop}_{\overline{\rm MS}} = 0.1$. It is customary to interpret $r_0 = 0.5$ fm when comparing this scale to one of the real world. Roughly, the potential shape in the displayed range $r < r_0/2$ accounts for formation of the $\Upsilon(1S)$ state. We plot three lines with the scale choices $\Lambda^{\rm 3\text{-}loop}_{\overline{\rm MS}}/\mu = 0.14$, 0.07, and 0.035. [The corresponding values of $\alpha_S(\mu)$ are 0.216, 0.165, and 0.135, respectively.] There is a small but visible dependence on the scale. The level of agreement with the lattice data shows that our prediction of the potential at this order is good enough to warrant quantitative description of the nature of the $\Upsilon(1S)$ state. We confirm the observation that, as we include higher-order corrections, agreement of the perturbative prediction and lattice computations improves up to larger distances. According to the analyses in [14,19], we anticipate that the agreement would get even better if we resum logarithms via RG, or appropriately choose the scale μ as a function of r, provided that the IR renormalon is subtracted.

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Note added.—Shortly after we announced our result, a paper by A. V. Smirnov *et al.* [31] appeared, which performed an independent computation of $\tilde{a}_3^{(0)}$. The results of the two Letters agree within the errors.

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