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 the computation of the static potential at this order.

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

Computations of $V_{\text{QCD}}(r)$ in perturbative QCD has a long history. At tree-level, $V_{\text{QCD}}(r)$ is merely a Coulomb potential, $-C_F q^2/r$ ($C_F = 4/3$ is a color factor), arising from one-gluon-exchange diagram. The 1-loop corrections (with massless and/or massive internal quarks) were computed in [1, 2]. The 2-loop correction (with massless internal quarks) was computed in [3]. The 2-loop correction due to massive internal quarks was computed in [4] (partly corrected in [5]). The logarithmic correction at 3-loop originating from the ultrasoft region, relevant to the bottomonium and charmonium states. In fact, the perturbative series turned out to be poorly convergent at $r > 0.1$ fm; uncertainty of the series for $r \rightarrow \infty$ is not optimal as the convergence of perturbative series is worse at larger $r$; rather it is better to fix $V_{\text{QCD}}(r)$ at some small distance. As it turned out, $V_{\text{QCD}}(r)$ becomes steeper at $r > 0.1$ fm as the order of the expansion is raised, hence convergence of perturbative series becomes worse if we fix $V_{\text{QCD}}(r)$ at $r \rightarrow \infty$. 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 $\alpha_s$. In fact, several studies have shown that perturbative predictions for $V_{\text{QCD}}(r)$ agree well with phenomenological potentials and lattice calculations of $V_{\text{QCD}}(r)$ in the intermediate distance region [3, 13, 14, 15].

The improvement of the situation opened up vast applications of the QCD potential in heavy quarkonium physics [16]. For instance, higher–order computations of $V_{\text{QCD}}(r)$ 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 3–loop correction to $V_{\text{QCD}}(r)$ 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 [17]. Another application is a precise determination of $\alpha_s$, from comparison of the perturbative prediction and lattice computations of $V_{\text{QCD}}(r)$ [18].

The static QCD potential is defined from an expecta-
tion value of the Wilson loop as

\[ V_{\text{QCD}}(r) = -\lim_{T \to \infty} \frac{1}{iT} \ln \left( \frac{0}{0} \right) \text{Tr} P e^{i \hat{H} T} A_\mu \left| 0 \right> \]

\[ = \left( \frac{\mu^2 e^{\gamma_E}}{4\pi} \right)^\epsilon \int \frac{d^4 q}{(2\pi)^4} e^{iq \cdot r} \left[ -4\pi C_F \alpha_V(q)^2 \right] \tag{1} \]

where \( q = \tilde{q} \); \( C \) 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. In this IR divergence is absent and regularized by the energy difference between color–singlet and octet intermediate states. The difference between \( V_{\text{QCD}}(r) \) and its perturbative expansion \( [V_{\text{QCD}}(r)]_{\text{PT}} \) can be treated systematically within the effective field theory “potential non–relativistic QCD” [19]. \( [V_{\text{QCD}}(r)]_{\text{PT}} \) is obtained from \( V_{\text{QCD}}(r) \) if we replace \( \alpha_V(q) \) in eq. \( 1 \) by \( \alpha_V^\text{PT}(q) \). This difference

\[ [V_{\text{QCD}}(r)]_{\text{US}} = V_{\text{QCD}}(r) - [V_{\text{QCD}}(r)]_{\text{PT}} \tag{7} \]

given by contributions of ultra–soft (US) degrees of freedom. In the region \( r < \Lambda_{QCD} \), the leading–order contribution to \( [V_{\text{QCD}}(r)]_{\text{US}} \) in double expansion in \( \alpha_S \) and \( \log(\alpha_S) \) is readily obtained from the result of [7] as

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

Upon Fourier transform, \( 1/\epsilon \) and \( \log \mu \) terms of eqs. [9] and [10] cancel each other. In general, at \( r < \Lambda_{QCD} \), one may perform operator–product–expansion of \( [V_{\text{QCD}}(r)]_{\text{US}} \) as multi–pole expansion in \( r \). In this case, non–perturbative contributions to \( [V_{\text{QCD}}(r)]_{\text{US}} \) are parametrized in the form of non–local gluon condensates.

We may classify \( \bar{a}_3 \) in [8] according to the powers of the number of flavors \( n_f \) of the internal quarks:

\[ \bar{a}_3 = n_f^3 \bar{a}_3^{(3)} + n_f^2 \bar{a}_3^{(2)} + n_f \bar{a}_3^{(1)} + \bar{a}_3^{(0)}. \tag{9} \]

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

Let us describe our calculational procedure. At tree–level and at 1–loop order, computation for \( [V_{\text{QCD}}(r)]_{\text{PT}} \) is more or less trivial. The 2–loop correction to \( [V_{\text{QCD}}(r)]_{\text{PT}} \) is expressed in terms of 5 master integrals, all of which are expressed in terms of \( \Gamma \) function and rational functions of \( \epsilon \) [20]. Hence, we may easily obtain expansion coefficients in \( \epsilon \) necessary for the 3–loop computation.

We first generate 3-loop Feynman diagrams for the scattering of static quark and antiquark using GRACE [21] and QGRAF [22]. There are about 20,000 diagrams; we confirmed that the diagrams generated by the two programs coincide. Next step is to eliminate iterations of the lower–order potential at the diagram level, which includes appropriate rearrangements of color factors associated with diagrams; we use the general algorithm developed in [23]. This procedure eliminates diagrams which contain pinch singularities. Subsequently the color factor for each diagram is simplified using the program color provided in [24].

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 computation, we collect integrands with a common denominator and cancel numerators against denominators as much as possible, by
appropriately expressing numerators in combinations of factors in the denominator. After these processes, we were able to express the 3–loop correction to $[V_{\text{QCD}}(r)]_{\text{PT}}$ 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 [25]. To carry out the reduction efficiently, we use the Laporta algorithm [26]. 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. 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 3–loop correction to $[V_{\text{QCD}}(r)]_{\text{PT}}$ is expressed in terms of about 1700 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 $\Gamma$ function and rational functions of $D$. The rest of the master integrals are expanded in Laurent series in $\epsilon$ 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) to evaluate Feynman parameter integrals using sector decomposition, and (b) to evaluate integrals in Mellin-Barnes representation. Typical relative accuracy in numerical evaluation of the expansion coefficients is of order $10^{-5}$. Details of our computation will be described elsewhere.

Our final result reads

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

with the color factor $d_F^{abcd}d_A^{abcd} / N_A = N_c(N_c^2+6)/48$ [22]. For completeness, we combine our result with that of [10] and list the numerical values of $\hat{a}_3$, defined in eq. (9), for $N_c = 3$ and $n_l = 3, 4, 5$ in Tab. 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 the QCD potential with the known renormalization constant of the strong coupling constant, as well as reproduction of known IR divergence, provide non–trivial cross checks. We have reproduced $\hat{a}_3^{(1)}, \hat{a}_3^{(2)}$, and the coefficient of $C_F$ in $\hat{a}_3^{(1)}$ [10] analytically. We also computed the coefficients of $C_A$, $C_A C_F$ and $d_F^{abcd}d_A^{abcd} / N_A$ in $\hat{a}_3^{(1)}$ numerically and confirmed that our results agree with those of [10] within the estimated errors. The last comparison provides a strong cross check on 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 $\hat{a}_3^{(3)}, \hat{a}_3^{(2)}, \hat{a}_3^{(1)}$ except for a single coefficient.

Now we compute $V_{\text{QCD}}(r)$, as given by the sum of $[V_{\text{QCD}}(r)]_{\text{PT}}$ and $[V_{\text{QCD}}(r)]_{\text{US}}$, including all the corrections up to $O(\alpha_s^4)$ and $O(\alpha_s^4 \log \alpha_s)$. Namely we use the series expansion [22] up to $n = 3$ for the former and eq. (8) for the latter.

In Fig. 1(a) we plot our prediction for $V_{\text{QCD}}(r)$ in the distance region corresponding to (would-be) toponium

| $n_l$ | 3  | 4  | 5  |
|------|----|----|----|
| $\hat{a}_3$ | 5199(3) | 3160(3) | 1460(3) |

TABLE I: Numerical values of $\hat{a}_3$, defined in eq. (9), for different values of $n_l$.
states. 3 lines are plotted, corresponding to $\mu = 25$, 50 and 100 GeV, with $n_1 = 5$ and $\alpha_S(M_Z) = 0.1176$. We added a constant to each prediction such that it takes a common value at $r = 0.01$ GeV$^{-1}$. The difference of the 3 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 [14, 27]. Accordingly we set $n_1 = 0$. We used the central value of $r_0^{3\text{-loop}} = 0.574 \pm 0.042$ [18] to fix the relation between the lattice scale and $\Lambda_{\overline{\text{MS}}}^{3\text{-loop}}$, 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 $r = 0.1$. 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 3 lines with the scale choices $\Lambda_{\overline{\text{MS}}}^{3\text{-loop}}/\mu = 0.14$, 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 [13, 18], we anticipate that the agreement would get even better if we resum logarithms via RG, or, appropriately choose the scale $\mu$ as a function of $r$, provided that the IR renormalon is subtracted.

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