Corrections to quarkonium 1S energy level at $\mathcal{O}(\alpha_s^4 m)$ from non-instantaneous Coulomb vacuum polarization

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We calculate $\mathcal{O}(\alpha_s^4 m)$ and $\mathcal{O}(\alpha_s^2 m \log \alpha_s)$ corrections to the quarkonium 1S energy level analytically, which have been overlooked in recent studies. These are the contributions from one Coulomb-gluon exchange with the 1-loop vacuum polarization insertion. A part of the corrections was computed numerically some time ago; we correct its error.

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Heavy quarkonium systems, such as bottomonium and charmonium, provide an important testing ground for studies on physics and dynamics of QCD boundstates using non-relativistic boundstate theory based on perturbative QCD. Recently accuracy of the theoretical predictions has improved dramatically. This owes to the progress in computations of higher-order perturbative corrections and the discovery [1] of cancellation of leading renormalons in these systems. So far, impacts in related fields have been as follows. (1) The mass of the bottom quark in the $\overline{\text{MS}}$ scheme has been determined accurately from the $\Upsilon$ spectrum [2]. It has various important applications in $B$ physics. Also it posed tight constraints on some models beyond the Standard Model such as supersymmetric Grand Unified Theories [3]. (2) The bottomonium spectrum is reproduced reasonably well by perturbative QCD up to the $n = 3$ levels. A new physical picture on the composition of the bottomonium masses has been proposed on the basis of the calculation [4]. (3) After incorporating the renormalon cancellation, the perturbative static QCD potential is shown to agree well with potentials of phenomenological models and with the QCD potential computed by lattice simulations [5].

Despite of these developments, in the context of non-relativistic boundstate theory, there have been no systematic methods for identifying higher-order corrections to physical quantities of heavy quarkonia (energy levels, decay rates, etc.) in the non-relativistic expansion in $1/c$ ($c$ is the speed of light). Rather, experts have identified separate contributions from inspections. A first attempt to compute $\mathcal{O}(1/c^2)$ corrections to the quarkonium energy levels was given in [6], although its main results contain errors [7]. In terms of the (effective) non-relativistic Hamiltonian for quarkonium systems, different terms up to $\mathcal{O}(1/c^2)$ have been identified as follows. The part which is identical with that for QED boundstates has been known for a long time (the Breit Hamiltonian). The 1-loop correction to the static QCD potential was computed in [8]; the 2-loop correction was calculated in [9].

The 1-loop correction to the static QCD potential was computed in [8] and the 2-loop correction was calculated in [9]. These corrections are from the ultra-soft region $k_0, |\vec{k}| \sim \alpha_s^2 m$ of the momentum of the gluon exchanged between quark ($Q$) and antiquark ($\bar{Q}$). From further inspections, we find corrections to the energy level at $\mathcal{O}(\alpha_s^4 m \log \alpha_s)$ and $\mathcal{O}(\alpha_s^2 m)$ originating from the ultra-soft and the soft momentum region $k_0, |\vec{k}| \sim \alpha_S m$. Both of these corrections stem from the non-instantaneous nature of the gluon vacuum polarization. In this paper we compute these corrections to the energy level of the quarkonium 1S state analytically in Coulomb gauge (see Fig. [1]). We assume that $Q$ and $\bar{Q}$
have equal masses. The gluonic contribution corresponds to the correction $\Delta^a M_{1S}$ computed numerically in [3].

Following [3], our computation of the perturbative corrections is based on the Bethe-Salpeter (BS) formalism [12]. We work in Coulomb gauge, since severe gauge cancellations occur in other gauges [24]. (Most computations in non-relativistic boundstate problems have been carried out in Coulomb gauge conventionally, except where gauge-independent contributions have been computed.) According to the BS formalism, the potential energy $E_{\text{pot}}$ and the self-energy contributions $E_{\text{SE}}$ in the total energy of the boundstate can be expressed, in the rest frame of the boundstate, as

$$E_{\text{pot}} = \frac{i}{2M} (\chi \cdot K \cdot \chi),$$

$$E_{\text{SE}} = M - \frac{i}{2M} (\chi \cdot [(S_F \chi)^{-1} (S_F \chi)^{-1}] \cdot \chi).$$

Here, $\chi, \chi$ and $K$ denote the BS wave functions and the BS-kernel, respectively; $M$ is the boundstate mass (total energy); $S_F$ represents the full propagator of $Q$ or $\bar{Q}$. We set the momentum of the center of gravity as $(M, 0)$. The dot (·) represents contraction of spinor indices and an integral over the relative momentum between $Q$ and $\bar{Q}$. Diagrammatically, $E_{\text{pot}}$ ($E_{\text{SE}}$) represents the contributions from the diagrams where the $Q$ and $\bar{Q}$ lines are connected (disconnected), and $E_{\text{pot}} + E_{\text{SE}} = M$.

We compute the contribution to the potential energy from the 1-loop vacuum polarization of the Coulomb gluon $\Pi(k)$:

$$\delta E_{\text{pot}}^{(1S)} = \left\langle \Pi(k) \right\rangle_{1S}$$

$$= \frac{i}{2M_{1S}^{(0)}} \int \frac{d^4p}{(2\pi)^4} \int \frac{d^4k}{(2\pi)^4} \int \frac{d^4q}{(2\pi)^4} \chi_{1S}^{(0)}(p)K_C(k)\Pi(k)\chi_{1S}^{(0)}(p + k).$$

This is shown diagrammatically in Fig. [1]. We assume that the quarks in the vacuum polarization are massless and compute $\delta E_{\text{pot}}^{(1S)}$ in a series expansion in $\alpha_S$ up to $O(\alpha^3_S m)$ and $O(\alpha^3_S m \log \alpha_S)$. In Eq. (3), $K_C = -i C_F (4 \pi \alpha_S m / |k|^2)(\gamma^0 \otimes \gamma^0)$ is the kernel of one Coulomb-gluon exchange at tree level. Throughout this paper $\alpha_S \equiv \alpha_S(\mu)$ denotes the strong coupling constant defined in the $\overline{\text{MS}}$ scheme with $n_f$ active flavors, where $\mu$ is the renormalization scale; $C_F$ is the Casimir operator of the fundamental representation of the color $SU(3)$ group. The BS wave functions in the leading-order of $1/c$-expansion are given by

$$\chi_{1S}^{(0)}(p) = [D(p) + D(-p)] \sqrt{2M_{1S}^{(0)}} \phi_{C,1S}(p) \lambda,$$

$$\overline{\chi}_{1S}^{(0)}(p) = [D(p) + D(-p)] \sqrt{2M_{1S}^{(0)}} \phi_{C,1S}(p) \lambda^\dagger,$$

$$D(p) = \frac{i}{M_{1S}^{(0)} / 2 + p_0 - m - \vec{p}^2 / 2m + i0},$$

Here, $m$ denotes the pole mass of $Q$ and $\bar{Q}$. $\phi_{C,1S}(p)$ and $M_{1S}^{(0)}$ denote the $1S$ Coulomb wave function and its energy level, respectively:

$$\phi_{C,1S}(p) = \frac{\sqrt{2\pi} (C_F \alpha_S m)^{3/2}}{[p^2 + (C_F \alpha_S m / g^2)]^{3/2}},$$

$$M_{1S}^{(0)} = 2m - \frac{(C_F \alpha_S m)^2}{4} m.$$

$\lambda$ represents the spin of the boundstate,

$$\lambda_J = \frac{1 + \gamma^0}{2} \sigma_J - \frac{1 - \gamma^0}{2},$$

where $\sigma_J = \gamma_5 \sqrt{2} / 2$ for $J = 0$ and $\sigma_J = \gamma_5 \sqrt{2} / 2$ for $J = 1$ and polarization vector $\epsilon$.

First we compute $\Pi(k)$ using dimensional regularization and in the $\overline{\text{MS}}$ renormalization scheme. (We assume that spacetime contains one time dimension and $3 - 2\epsilon$ space dimensions.) The Feynman diagrams contributing to $\Pi(k)$ are shown in Fig. [2]. Since this is a 1-loop calculation, it can be carried out more or less straightforwardly. Some useful techniques for calculations in Coulomb gauge with dimensional regularization can be found in [25]. We write

$$\Pi(k) = \frac{\alpha_S}{4\pi} \left[ C_A \Pi_g(k) + T_R n_f \Pi_q(k) \right],$$

where $C_A$ is the Casimir operator of the adjoint representation and $T_R$ is the trace normalization of the fundamental representation. We obtain the gluon contribution:

$$\Pi_g(k) = -\frac{11}{3\epsilon} + \Gamma(\epsilon) e^{\gamma_E} \left( \frac{\mu^2}{|k|^2} \right)^\epsilon$$

$$\times \left[ 2 \Gamma(1 - \epsilon) \Gamma(\frac{3}{2} - \epsilon) + 2 (5 - 4 \epsilon) \Gamma(2 - \epsilon)^2 (1 - \rho^2)^{3/2} \Gamma(4 - 2\epsilon) \right]$$

$$+ \epsilon \left[ 2 + \gamma^0 \{2 (3 - 2\epsilon) \} K(\epsilon, \rho) \right]$$

$$= \frac{11}{3} \log \left( \frac{\mu^2}{|k|^2} \right) - \frac{8}{3} \log(1 - \rho^2) + \frac{31}{9} + \log(\epsilon),$$

$$+ \frac{1}{3} \log \left( \frac{\mu^2}{|k|^2} \right) - 8 \log(1 - \rho^2) + 3f(\rho) + f(\rho) \left[ 3 \log(1 - \rho^2) - 12 \log 2 + 6 - 3f(\rho) \right] + O(\epsilon),$$

$$+ \frac{1}{3} \log \left( \frac{\mu^2}{|k|^2} \right) - 8 \log(1 - \rho^2) + 3f(\rho) + f(\rho) \left[ 3 \log(1 - \rho^2) - 12 \log 2 + 6 - 3f(\rho) \right] + O(\epsilon).$$
where $\rho = k_0/|\vec{k}|$, and
\[K(\rho, \rho) = \int_0^1 dx \int_0^1 dy \frac{x^{1-\varepsilon} y^{1-\varepsilon}}{((1-x)y - (1-x)\rho^2)^{1+\varepsilon}},\] (13)
\[f(\rho) = \frac{1-\rho^2}{\rho} \left[ L_2 \left( \frac{1-\rho}{1+\rho} \right) + \frac{\log^2 \left( 1+\rho \right) - \pi^2}{12} \right] - 2 \log 2.\] (14)
The analytic expression (12) is a new result. On the other hand, the contribution from a massless quark is gauge independent and well known:
\[\Pi_q(k) = \frac{4}{3} \zeta(1+\varepsilon) \frac{\mu^2}{k^2 - \varepsilon} \frac{8\Gamma(2-\varepsilon)^2}{\Gamma(4-2\varepsilon)}\] (15)
\[= -\frac{4}{3} \log \left( \frac{\mu^2}{k^2} \right) - \frac{20}{9} \log \varepsilon + O(\varepsilon).\] (16)

For $k_0^2 > |\vec{k}|^2$ the vacuum polarization $\Pi(k)$ acquires an imaginary part; in this case, the usual $+i0$ prescription, $k_0^2 \rightarrow k_0^2 + i0$, is understood. If we take the instantaneous limit $k_0 \rightarrow 0$ of the Coulomb propagator $-C_F(4\pi\alpha_S/|\vec{k}|^2)[1 + \Pi(k)]$, the 1-loop static QCD potential in momentum space [2] is correctly reproduced. It is ensured by the Ward identity in Coulomb gauge [22].

Next we evaluate the integral (1). One may easily verify that the integral is finite both in ultraviolet and infrared regions. Using the expressions (11), (13) and (12) for $\Pi(k)$, we may take advantage of the functions $J(\varepsilon)$ and $I(\varepsilon, \Delta)$ analyzed in [18]. These functions are defined similarly to $\delta E_{\text{pot}}^{(1S)}$, where $\Pi(k)$ is replaced by $|\vec{k}|^{-2\varepsilon}$ or by $(-\xi^2k_0^2 + |\vec{k}|^2 - i0)^{-\varepsilon}$ in Eq. (1):
\[\left\langle |\vec{k}|^{-2\varepsilon} \right\rangle_{1S} = \frac{(C_F\alpha_S)^2}{2} \frac{m}{(C_F\alpha_S m)^{-2\varepsilon}} J(\varepsilon),\]
\[\left\langle (-\xi^2k_0^2 + |\vec{k}|^2 - i0)^{-\varepsilon} \right\rangle_{1S} = \frac{(C_F\alpha_S)^2}{2} \frac{m}{(C_F\alpha_S m)^{-2\varepsilon}} I(\varepsilon, \xi \Delta).\] (17)

Here, $\Delta = C_F\alpha_S/2$ represents the ratio of the Coulomb binding energy and the Bohr scale. Then $\delta E_{\text{pot}}^{(1S)}$ can be expressed in terms of $I(\varepsilon, \Delta)$ and $J(\varepsilon)$ plus an integral over $x$ and $y$ of terms involving $I(\varepsilon, \sqrt{1-xy})$ and its derivative with respect to $\Delta$. In order to obtain the series expansion of $\delta E_{\text{pot}}^{(1S)}$ in $\alpha_S$, it suffices to replace $I(\varepsilon, \Delta)$ by its asymptotic expansion in $\Delta$ given by
\[I(\varepsilon, \Delta) = I_{\text{pot}}^{(0)}(\varepsilon) + \Delta \cdot I_{\text{pot}}^{(1)}(\varepsilon) + \Delta^{1-2\varepsilon} \cdot I_{\text{pot}}^{(2)}(\varepsilon) + \cdots.\] (18)

Only those terms relevant to our calculation are written explicitly. $I_{\text{pot}}^{(0)}$ and $I_{\text{pot}}^{(1)}$ were given in [18], while $I_{\text{pot}}^{(1)}$ is needed additionally:
\[I_{\text{pot}}^{(1)}(\varepsilon) = 4\pi^{-3/2} \Gamma(1 - \varepsilon) \Gamma(\frac{1}{2} + \varepsilon).\] (19)

The integral over $x$ and $y$ can be evaluated analytically. We obtain
\[\delta E_{\text{pot}}^{(1S)} = -\frac{1}{4} \left( C_F\alpha_S \right)^2 m\]
\[\times \left[ \left( \frac{\alpha_S}{\pi} \right) C_A \tilde{d}_g^{(1)} + TR_{l_1} d_{g}^{(1)} \right.\]
\[+ \left( \frac{\alpha_S}{\pi} \right)^2 \left( C_A C_F d_g^{(2)} + TR_{l_1} C_F d_{g}^{(2)} \right) + \mathcal{O}(\alpha_S^3) \right]\] (20)
with
\[d_g^{(1)} = \frac{11}{3} \log \left( \frac{\mu}{C_F\alpha_S m} \right) + \frac{97}{18},\] (21)
\[d_q^{(1)} = -\frac{4}{3} \log \left( \frac{\mu}{C_F\alpha_S m} \right) - \frac{22}{9},\] (22)
\[d_q^{(2)} = \left( \frac{28}{3} - \pi^2 \right) \log(C_F\alpha_S) - 10 + \frac{\pi^2}{4} + 7\xi,\] (23)
\[d_q^{(2)} = -\frac{8}{3} \log(C_F\alpha_S) + 4.\] (24)

The $\mathcal{O}(\alpha_S^3)$ terms $[d_g^{(1)}$ and $d_q^{(1)}]$, stem from the static QCD potential and are well known. The $\mathcal{O}(\alpha_S^4m)$ terms $[d_g^{(2)}$ and $d_q^{(2)}]$ are the new results. We made a cross check of our results through an independent computation using a different integral representation of $\Pi(k)$ and a slightly generalized version of the function $I(\varepsilon, \Delta)$. We also checked our results by calculating the momentum-space integral (3) numerically.

One may use the threshold expansion technique [13] in order to clarify from which kinematical regions individual perturbative corrections originate. We confirmed that, with respect to the quark-loop contribution, the potential region $(k_0 \sim \alpha_S^2 m, |\vec{k}| \sim \alpha_S m)$ accounts for $d_g^{(1)}$, the soft region induces $-\left( 8/3 \right) \log(\mu/[2C_F\alpha_S m])$ plus a constant; the ultra-soft region induces $+\left( 8/3 \right) \log(\mu/[2C_F^2\alpha_S^2 m])$ plus a constant; the latter two contributions add up to produce $d_g^{(2)}$. Similar separate contributions can be identified also for the gluonic contribution.

As stated, the gluonic contribution $d_g^{(2)}$ was computed numerically in [4]. Comparing our result with the numerical results listed in TABLE I of that paper, we find that their results for the $1S$ state are smaller than ours by about factor 6, consistently for all the listed values of $\alpha_s$. 

![Feynman diagrams](image-url) FIG. 2: Feynman diagrams for the 1-loop Coulomb vacuum polarization: (a) massless quark loop, (b) transverse-Coulomb gluon (\(g_T-g_T\)) loop, and (c)(d) transverse gluon loops.
\begin{table}
\begin{tabular}{|c|c|}
\hline
$C_A C_F d_{Q}^{(2)}$ & $3.5 - 2.1 \log(C_F a_S)$ \\
\hline
$T_R n_1 C_F d_{Q}^{(2)}$ & $10.7 - 7.1 \log(C_F a_S)$ \\

\hline
$A_{QCD\text{pot}}$ & $153.6 + 119.1 \ell + 52.1 \ell^2$ \\
\hline
$A_{1/\ell^2}$ & 39.5 \\
$A_{\text{Breit}}(J = 1)$ & $-0.4$ \\
$A_{\text{Breit}}(J = 0)$ & 23.0 \\
\hline
\end{tabular}
\caption{A numerical comparison of our results with the previously known corrections at $O(a_S^2 \mu)$. We take $n_1 = 4$, $\ell = \log[\mu/(C_F a_S \mu)]$.}
\end{table}

$\alpha_S$. (Note that $\alpha_S$ in \cite{3} should read $C_F a_S$ in contemporary notations.) We have checked that Eq. (5.13) of that paper is correct. Therefore, we suspect that some error has occurred in transforming this equation to the final results given in the table of that paper. We are unable to locate the error more precisely, since no details are provided for this part of the computation.

Let us compare our results with the other $O(a_S^2 \mu)$ corrections:

$$\delta E_{1/2} = -\frac{1}{4} \left( C_F a_S \right)^2 m \times \left( \frac{\alpha_S}{\pi} \right)^2 \times (A_{QCD\text{pot}} + A_{1/\ell^2} + A_{\text{Breit}}). \quad (25)$$

We separate the corrections into 3 parts: $A_{QCD\text{pot}}$ denotes the correction originating from the static QCD potential; $A_{1/\ell^2}$ denotes the correction originating from the $\omega C_F a_S^2/(2m^2)$ potential; $A_{\text{Breit}}$ denotes the correction originating from the Breit Hamiltonian. A numerical comparison is given in Table I for $n_1 = 4$ and for the standard values of the color factors $C_F = 4/3$, $C_A = 3$ and $T_R = 1/2$. We see that the corrections $C_A C_F d_{Q}^{(2)}$ and $T_R n_1 C_F d_{Q}^{(2)}$ are not negligible as compared to $A_{1/\ell^2}$ or $A_{\text{Breit}}$, whereas $A_{QCD\text{pot}}$ is an order of magnitude larger than the other corrections (for a typical choice of $\mu$) due to an enhancement by $O(\Lambda_{QCD})$ renormalon \cite{23}.

The reason why the corrections calculated here have been overlooked in the effective theories appears to be two-fold: (1) The present power counting schemes cannot specify all diagrams (and kinematical regions) which contribute to a given order of $1/\epsilon$ expansion. (2) The effective theories have been matched to on-shell $QQ$ amplitudes of perturbative QCD; generally the matching should be performed with off-shell $QQ$ amplitudes or including on-shell amplitudes with additional gluons in external lines \cite{24}. We consider that we have not yet understood well higher-order corrections in the non-relativistic boundstate theory, especially where the soft and ultraviolet contributions are involved.

Our results given here also apply to the QED boundstates composed of heavy particles such as the $\mu^+\mu^-$ boundstate, after trivial replacements of the color factors and the coupling constant.

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