Next-to-next-to-leading order vacuum polarization function of heavy quark near threshold and sum rules for $b\bar{b}$ system.

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Abstract

A correlator of the vector current of a heavy quark is computed analytically near threshold in the next-to-next-to-leading order in perturbative and relativistic expansion that includes $\alpha_s^2$, $\alpha_s v$ and $v^2$ corrections in the coupling constant and velocity of the heavy quark to the nonrelativistic Coulomb approximation. Based on this result, the numerical values of the $b$-quark pole mass and the strong coupling constant are determined from the analysis of sum rules for the $\Upsilon$ system. The next-to-next-to-leading corrections are found to be of order of next-to-leading ones.

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Insufficiency of the ordinary PT for description the near threshold behavior of vacuum polarization function was noted long ago in the context of Coulombic resummation in nonrelativistic QED [1, 2]. Recently a considerable progress has been made in studying the near threshold production of heavy quark-antiquark pair within perturbation theory of QCD with resummation of threshold singularities. Both perturbative and relativistic corrections have been taken into account in the next-to-next-to-leading order in the coupling constant and velocity of the heavy quark to the leading nonrelativistic approximation based on Coulomb potential [3, 4, 5]. This theoretical development provides more accurate description of the heavy quark vacuum polarization function in the threshold region necessary for such applications as the top quark production [6] and the precise quantitative investigation of the Υ system [7, 8]. In the latter case higher order corrections to leading Coulomb behavior in the threshold region are essential both numerically for extracting the $b$-quark mass and the strong coupling constant [3] and qualitatively for justifying the perturbative expansion around Coulomb solution. The analytical calculation of the next-to-next-to-leading order corrections has not been completed yet though some results are available [1].

In this paper we present the complete analytical expression for a correlator of the vector current of heavy quarks near threshold in the next-to-next-to-leading order resumming all $\mathcal{O}[(\alpha_s/v)^n \times (\alpha_s^2, \alpha_s v, v^2)]$ terms, with $v$ being the heavy quark velocity. The correlator is further used for determination of the bottom quark pole mass $m_b$ and the strong coupling constant $\alpha_s$ from sum rules for the Υ system.

We study the near threshold behavior of the polarization function $\Pi(s)$ of the $b$-quark vector current $j_\mu = \bar{b}\gamma_\mu b$

$$\left(q_\mu q_\nu - g_\mu\nu q^2\right) \Pi(q^2) = i \int dx e^{ixq} \langle 0 | T j_\mu(x) j_\nu(0) | 0 \rangle$$

within the nonrelativistic expansion [9] which in the next-to-next-to-leading order

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1 Semi-analytical analysis of the complete next-to-next-to-leading order corrections to the heavy quark polarization function near the two-particle threshold has been done in the context of the photon mediated $t$ quark pair production [4, 5].
reads
\[
\Pi(s) = \frac{N_c}{2m_b^2} \left( C_h(\alpha_s)G(0,0,k) + \frac{4}{3} \frac{k^2}{m_b^2} G_C(0,0,k) \right) \tag{1}
\]
with \( k = \sqrt{m_b^2 - \frac{s}{4}} \) being a natural energy variable near threshold. First term in brackets gives the representation for the correlator within NRQC D with \( C_h(\alpha_s) \) being a perturbative coefficient matching correlators of relativistic and nonrelativistic vector currents. The coefficient \( C_h(\alpha_s) \) is computable in full QCD and by now is known to the second order in \( \alpha_s \) expansion
\[
C_h(\alpha_s) = 1 - C_1^h C_F \frac{\alpha_s}{\pi} + C_2^h C_F \left( \frac{\alpha_s}{\pi} \right)^2
\]
with \( C_1^h = 4 \) and
\[
C_2^h = \left( \frac{39}{4} - \frac{\zeta(3)}{3} + \frac{4\pi^2}{3} \ln 2 - \frac{35\pi^2}{18} \right) C_F - \left( \frac{151}{36} + \frac{13}{2} \zeta(3) + \frac{8\pi^2}{3} \ln 2 - \frac{179\pi^2}{72} \right) C_A
\]
\[
+ \left( \frac{44}{9} - \frac{4\pi^2}{9} + \frac{11}{9} n_f \right) T_F + 2 \left( \beta_0 + \frac{\pi^2}{3} C_F + \frac{\pi^2}{2} C_A \right) \ln \left( \frac{m_b}{\mu} \right) \tag{2}
\]
in \( \overline{\text{MS}} \) renormalization scheme \([4,5,11]\). Here the group invariants for QCD are \( C_A = 3, C_F = 4/3, T_F = 1/2, \) and \( \gamma_E = 0.577216 \ldots \) is the Euler constant, \( \zeta(z) \) is the Riemann \( \zeta \)-function, \( n_f \) is the number of light flavors, and \( \beta_0 = 11C_A/3 - 4T_F n_f/3 \). The quantity \( G(x,y,k) \) is the nonrelativistic Green function (GF) of the following Schrödinger equation
\[
\left( -\frac{\Delta_x}{m_b} - \frac{\Delta_y^2}{4m_b^2} + V_C(x) + \frac{\alpha_s}{4\pi} V_1(x) + \left( \frac{\alpha_s}{4\pi} \right)^2 V_2(x) \right)
\]
\[
+ V_{NA}(x) + V_{BF}(x,y) + \frac{k^2}{m_b} \right) G(x,y,k) = \delta(x-y) \tag{3}
\]
where \( V_C(x) = -C_F \alpha_s/x \) is the Coulomb potential which is supposed to dominate the whole QCD interaction in the energy region of interest, \( x = |x|, V_{NA}(x) = -C_A C_F \alpha_s^2/(m_b x^2) \) is the non-Abelian potential of quark-antiquark interaction \([12]\), \( V_{BF}(x,y) \) is the standard Breit-Fermi potential (up to the color factor \( C_F \)) containing the quark spin operator \( s \), \textit{e.g.} \([13]\). The terms \( V_i \ (i = 1, 2) \) represent first and second order perturbative QCD corrections to the Coulomb potential \([14,15]\)
\[
V_1(x) = V_C(x) (C_0^1 + C_1^1 \ln(x\mu)),
\]
\[ V_2(x) = V_C(x)(C_0^2 + C_1^2 \ln(x\mu) + C_2^2 \ln^2(x\mu)), \]  
(4)

where

\[ C_0^1 = a_1 + 2\beta_0 \gamma_E, \quad C_0^1 = 2\beta_0, \]
\[ C_0^2 = \left( \frac{\pi^2}{3} + 4\gamma_E^2 \right) \beta_0^2 + 2(\beta_1 + 2\beta_0 a_1)\gamma_E + a_2, \]
\[ C_1^2 = 2(\beta_1 + 2\beta_0 a_1) + 8\beta_0^2 \gamma_E, \quad C_2^2 = 4\beta_0^2, \]
\[ a_1 = \frac{31}{9} C_A - \frac{20}{9} T_{Fn_f}, \]
\[ a_2 = \left( \frac{4343}{162} + 6\pi^2 - \frac{\pi^4}{4} + \frac{22}{3} \zeta(3) \right) C_0^2 - \left( \frac{1798}{81} + \frac{56}{3} \zeta(3) \right) C_A T_{Fn_f} \]
\[ - \left( \frac{55}{3} - 16\zeta(3) \right) C_F T_{Fn_f} \left( \frac{20}{9} T_{Fn_f} \right)^2, \]
\[ \beta_1 = \frac{34}{3} C_A^2 - \frac{20}{3} C_A T_{Fn_f} - 4C_F T_{ Fn_f}. \]

The second term in eq. (4) is generated by the operator of dimension four in the nonrelativistic expansion of the vector current (see, for example, \[16\]). It contains the GF of the pure Coulomb Schrödinger equation \[17\] at the origin

\[ G_C(0, 0, k) = -\frac{C_F\alpha_s b}{4\pi} \left( \frac{k}{C_F\alpha_s m_b} + \ln \left( \frac{k}{\mu} \right) + \gamma_E + \Psi_1 \left( 1 - \frac{C_F\alpha_s m_b}{2k} \right) \right), \]
(5)

where \( \Psi_1(x) = \Gamma'(x)/\Gamma(x) \) and \( \Gamma(x) \) is the Euler \( \Gamma \)-function.

The solution to eq. (3) can be found within the standard nonrelativistic perturbation theory around the Coulomb GF \( G_C(x, y, k) \). The leading order corrections to the Coulomb GF at the origin due to \( \Delta^2, V_{NA} \) and \( V_{BF} \) terms are known analytically \[4, 5\]. After including these corrections the approximate GF of eq. (3) at the origin takes the form \[4\]

\[ G(0, 0, k) = -\frac{C_F\alpha_s b}{4\pi} \left( \left( 1 - \frac{5}{8} \frac{k^2}{m_b^2} \right) \frac{k}{C_F\alpha_s m_b} + \left( 1 - 2 \frac{k^2}{m_b^2} \right) \right) \]
\[ \left( \ln \left( \frac{k}{\mu} \right) + \gamma_E + \Psi_1 \left( 1 - \frac{C_F\alpha_s m_b}{2k} \right) \right) \]
\[ + \frac{11}{16} \frac{C_F\alpha_s k}{m_b} \Psi_2 \left( 1 - \frac{C_F\alpha_s m_b}{2k} \right) \]
(6)

\[ \text{The term } V_{NA} \text{ can be fully accounted for the Coulomb GF because the corresponding differential equation is exactly solvable in standard special functions. Numerically this is not important for applications though.} \]
where $\Psi_2(x) = \Psi'_1(x)$. Note that in ref. [4] the shift of the spectrum of intermediate nonrelativistic Coulomb bound states was treated exactly i.e. without expanding of the energy denominators. This accounts for a part of the higher order corrections. We, however, consistently work in the next-to-next-to-leading order and keep only the second order terms in eq. (6). Since this part of the corrections is relatively small the difference between these two approaches is really negligible for the numerical analysis of the sum rules.

The correction $\Delta G_1$ to eq. (6) due to the first iteration of $V_1$ term of the QCD potential has been found in ref. [3] where the consistent analysis of sum rules for $b\bar{b}$ system in the next-to-leading order has been performed

$$\Delta G_1(0, 0, k) = \frac{\alpha_s}{4\pi} \frac{C_F \alpha_s m_b^2}{4\pi} \left( \sum_{m=0}^{\infty} F^2(m)(m+1) \left( C_0^1 + (L_k + \Psi_1(m+2))C_1^1 \right) \right.$$ 

$$-2 \sum_{m=1}^{\infty} \sum_{n=0}^{m-1} F(m)F(n) \frac{n+1}{m-n} C_1^1 + 2 \sum_{m=0}^{\infty} F(m) \left( C_0^1 + (L_k - 2\gamma_E - \Psi_1(m+1))C_1^1 \right)$$ 

$$+ L_k C_0^1 + \left( -\gamma_E L_k + \frac{1}{2} L_k^2 \right) C_1^1$$

(7)

where $L_k = \ln \left( \frac{\mu^2}{k} \right)$ and

$$F(m) = \frac{C_F \alpha_s m_b}{(m+1)2k} \left( m + 1 - \frac{C_F \alpha_s m_b}{2k} \right)^{-1}.$$ 

The correction $\Delta G_2^{(2)}$ to eq. (6) due to $V_2$ part of the potential is also known [3]

$$\Delta G_2^{(2)}(0, 0, k) = \left( \frac{\alpha_s}{4\pi} \right)^2 \frac{C_F \alpha_s m_b^2}{4\pi} \left( \sum_{m=0}^{\infty} F^2(m) \left( (m+1) \left( C_0^2 + L_k C_1^2 + L_k^2 C_2^2 \right) \right) \right.$$ 

$$+ (m+1)\Psi_1(m+2) \left( C_1^2 + 2L_k C_2^2 \right) + I(m)C_2^2$$ 

$$+ 2 \sum_{m=1}^{\infty} \sum_{n=0}^{m-1} F(m)F(n) \left( -\frac{n+1}{m-n} \left( C_1^2 + 2L_k C_2^2 \right) + J(m,n)C_2^2 \right)$$ 

$$+ 2 \sum_{m=0}^{\infty} F(m) \left( C_0^2 + L_k C_1^2 + (L_k^2 + K(m))C_2^2 - (2\gamma_E + \Psi_1(m+1)) \left( C_1^2 + 2L_k C_2^2 \right) \right)$$ 

$$+ L_k C_0^2 + \left( -\gamma_E L_k + \frac{1}{2} L_k^2 \right) C_1^2 + N(k)C_2^2$$

(8)
where
\[ I(m) = (m + 1) \left( \Psi_1^2(m + 2) - \Psi_2(m + 2) + \frac{\pi^2}{3} - \frac{2}{(m + 1)^2} \right) - 2(\Psi_1(m + 1) + \gamma_E), \]
\[ J(m, n) = 2 \frac{n + 1}{m - n} \left( \Psi_1(m - n) - \frac{1}{n + 1} + 2\gamma_E \right) + 2 \frac{m + 1}{m - n}(\Psi_1(m - n + 1) - \Psi_1(m + 1)), \]
\[ K(m) = 2(\Psi_1(m + 1) + \gamma_E)^2 + \Psi_2(m + 1) - \Psi_1^2(m + 1) + 2\gamma_E^2, \]
\[ N(k) = \left( \gamma_E + \frac{\pi^2}{6} \right)L_k - \gamma_EL_k^2 + \frac{1}{3}L_k^3. \]

In this paper we complete these results by computing the correction \( \Delta G_2^{(1)} \) due to the second iteration of \( V_1 \) term which of the proper (next-to-next-to-leading) order according to counting of smallness in nonrelativistic QCD with respect to \( \alpha_s \) and \( v \).

The result reads
\[ \Delta G_2^{(1)}(0, 0, k) = \left( \frac{\alpha_s}{4\pi} \right)^2 \frac{C_F\alpha_s}{4\pi} \frac{m_b^3}{2k} \left( \sum_{m=0}^{\infty} H^3(m)(m + 1) \left( C_0^1 + \Psi(m + 2) + L_k \right) C_1^1 \right)^2 \]
\[ -2 \sum_{m=1}^{\infty} \sum_{n=0}^{m-1} \frac{n + 1}{m - n} C_1^1 \left( H^2(m)H(n) \left( C_0^1 + \left( \Psi(m + 2) + L_k - \frac{1}{2} \frac{1}{m - n} \right) C_1^1 \right) \right. \]
\[ + H(m)H^2(n) \left( C_0^1 + \left( \Psi(n + 2) + L_k - \frac{1}{2} \frac{n + 1}{(m - n)(m + 1)} \right) C_1^1 \right) \right) \]
\[ + 2(C_1^1)^2 \left( \sum_{m=2}^{\infty} \sum_{n=1}^{m-1} \sum_{l=0}^{n+1} H(m)H(n)H(l) \frac{n + 1}{(l - n)(m - n)} \right. \]
\[ + \sum_{m=2}^{\infty} \sum_{n=1}^{m-1} \sum_{l=0}^{n-1} H(m)H(n)H(l) \frac{l + 1}{(n - l)(m - n)} \]
\[ + \sum_{n=2}^{\infty} \sum_{m=1}^{n-1} \sum_{l=0}^{m-1} H(m)H(n)H(l) \frac{(l + 1)(m + 1)}{(n + 1)(n - l)(n - m)} \right) \]

where
\[ H(m) = \left( m + 1 - \frac{C_F\alpha_s m_b}{2k} \right)^{-1}. \]

We are going to describe the details of this rather cumbersome calculation elsewhere.

One remark is in order though. Because ultraviolet divergences in eq. (6) depend on \( k \)
one has to match the calculation of these corrections to the calculation of the Wilson coefficient \( C_h(\alpha_s) \) (eq. (2)) \[4, 5\]. Such matching is not necessary for the calculation of \( \Delta G_1 \) and \( \Delta G_2^{(i)} \) terms because their divergent parts are \( k \) independent.

Thus eqs. (1, 5-9) give the complete analytical expressions for the vacuum polarization function of heavy quarks near the two-particle threshold in the next-to-next-to-leading order \( 3 \). Eqs. (5-9) look awkward and they can be rendered into more readable form by using \( \Psi \) functions for expressing some of the sums entering the formulae. However for direct numerical analysis of sum rules for \( b\bar{b} \) system this form is most suitable with respect to applicability of efficient numerical algorithms of a symbolic system.

Obtained formulae are applied to the analysis of the \( \Upsilon \) system for extraction of the \( b \)-quark pole mass \( m_b \) and the coupling constant \( \alpha_s \). The sum rules are formulated in the literature \[3, 8\] and we will use the latest version \[3\] with correct large \( n \) behavior.

The moments \( \mathcal{M}_n \)

\[
\mathcal{M}_n = \frac{12\pi^2}{n!} (4m_b^2)^n \left. \frac{d^n}{ds^n} \Pi(s) \right|_{s=0} = (4m_b^2)^n \int_0^\infty \frac{R(s)ds}{s^{n+1}}
\]

of the spectral density \( R(s) = 12\pi \text{Im}\Pi(s + i\epsilon) \) are compared with experimental ones

\[
\mathcal{M}_n^{\text{exp}} = \frac{(4m_b^2)^n}{Q_b^2} \int_0^\infty \frac{R_b(s)ds}{s^{n+1}}
\]

under the assumption of quark-hadron duality. The experimental moments \( \mathcal{M}_n^{\text{exp}} \) are generated by the function \( R_b(s) \) which is the normalized cross section \( R_b(s) = \sigma(e^+e^- \rightarrow \text{hadrons}_{\bar{b}b})/\sigma(e^+e^- \rightarrow \mu^+\mu^-) \). Here \( Q_b = -1/3 \) is the \( b \)-quark electric charge.

Numerical values are obtained basically by saturating the experimental moments with the contribution of the first six \( \Upsilon \) resonances (see \[3\] for details). Their leptonic widths \( \Gamma_k \) and masses \( M_k \) \( (k = 1 \ldots 6) \) are known with good accuracy \[18\]

\[
\mathcal{M}_n^{\text{exp}} = \frac{(4m_b^2)^n}{Q_b^2} \left( \frac{9\pi}{\alpha^2_{\text{QED}}(m_b)} \sum_{k=1}^6 \frac{\Gamma_k}{M_k^{2n+1}} + \int_0^\infty ds \frac{R_b(s)}{s^{n+1}} \right).
\]

\[3\] In refs. \[4, 5\] the corrections to the Coulomb GF due to \( V_i \) \( (i = 1, 2) \) terms of the potential were treated numerically for complex values of energy far from the real axis.
The rest of the spectrum beyond the resonance region for energies larger than \( s_0 \approx (11.2 \text{ GeV})^2 \) (continuum contribution) lies far from threshold and is safely approximated by the ordinary PT expression for the theoretical spectral density, so there \( R_b(s) \approx R(s) \). The influence of the continuum on high moments is almost negligible numerically and in any case under strict control\(^4\). Electromagnetic coupling constant is renormalized to the energy of order of \( m_b \) with the result \( \alpha^2_{\text{QED}}(m_b) = 1.07 \alpha^2 \) \(^8\).

We work with moments for \( 10 < n < 20 \) that simultaneously guarantees the smallness of both the continuum contribution and the nonperturbative power corrections due to the gluonic condensate \(^8\). The first one is not well known experimentally and has to be suppressed to make results independent of \( s_0 \). The second one should be small because the value of gluonic condensate (and higher order condensates) is not known well numerically. The normalization point \( \mu = m_b \) is used throughout the computation\(^4\). At the scale \( \mu = m_b \) both the hard and soft gluon corrections are of the same order of magnitude. For a lower scale the hard corrections become large while for higher scale the same is true for the soft corrections \(^3\). We found that at \( \mu \sim m_b \) the \( \mu \) dependence of the results is minimal which is a solid indication that at this point the higher order corrections are also small.

The result of the fit is

\[
\alpha_s(m_b) = 0.22 \pm 0.02, \quad \text{or} \quad \alpha_s(M_Z) = 0.118 \pm 0.006.
\]

The sum rules are much more sensitive to the \( b \)-quark mass than to the strong coupling constant so it is instructive to fix \( \alpha_s(M_Z) = 0.118 \) to the “world average” value \(^8\).

\(^4\) The expressions for the first few moments of the spectral density are now available in ordinary perturbation theory with \( \alpha_s^2 \) accuracy \(^9\), however, they cannot be used in theoretical formulas for sum rules directly because the spectrum is well known experimentally only for energies close to threshold due to existence of sharp resonances while the contribution of the continuum to these low moments is large in comparison with the resonance contribution.

\(^5\) We work strictly in the next-to-next-to-leading order approximation and, therefore, use the same normalization point for soft and hard corrections in contrast to \(^4\) \(^8\) where different normalization points were chosen for these two parts.
and then to extract \( m_b(n) \). In this way we obtain the following estimate for the mean value over the considered range of \( n \)

\[
m_b = 4.78 \text{ GeV}.
\]

This value is in a good agreement with the results of the first order analysis [3] where at \( \alpha_s(M_Z) = 0.118 \) we obtained

\[
m_b = 4.75 \text{ GeV}.
\]

Note that the optimization procedure [20] was used to improve convergence of perturbation theory in the previous analysis [3]. As we see this procedure turns out to be a powerful tool to estimate the higher order contributions. For comparison, the leading order result is \( m_b = 4.70 \) GeV and in the next-to-leading approximation without optimization one gets \( m_b = 4.72 \) GeV.

Main uncertainties of numerical values for considered parameters stem from the same sources that were identified in ref. [3]. The error coming from \( n \) distribution for the mass at fixed value of the coupling constant is about ±0.5% for \( 10 < n < 20 \). The \( \mu \) dependence for \( \mu = m_b ± 1 \text{ GeV} \) (where this dependence is minimal) introduces another ±0.5% of uncertainty. Thus our final estimate of the bottom quark pole mass is

\[
m_b = 4.78 ± 0.04 \text{ GeV}.
\]

Note that the uncertainty originated from the \( n \) and \( \mu \) dependence is not reduced in comparison with the next-to-leading order. This means that the contribution of the higher order corrections which has to cancel \( n \) and \( \mu \) dependence of the results is still important. Let us emphasize that the convergence of the perturbation theory for the vacuum polarization function of heavy quark near threshold is not fast.

We have found the next-to-next-to-leading order corrections to be of order of the next-to-leading ones. Furthermore, in the case of \( b \)-quark the corrections due to the perturbative modification of the Coulomb instantaneous potential (i.e. related
to $\Delta G_1$ and $\Delta G_2^{(i)}$ terms) dominate the total correction in the next-to-leading and next-to-next-to-leading orders. Inclusion of these corrections is quite important for consistent analysis of sum rules for the $\Upsilon$ system.

To conclude we have constructed an expression for the vacuum polarization function of the vector current of a heavy quark near threshold. It is completely analytic in the next-to-next-to-leading order in perturbative and relativistic expansion up to $\alpha_s^2, \alpha_s v$ and $v^2$ corrections. The polarization function was used for determination of the $b$-quark pole mass and the coupling constant from sum rules for the $\Upsilon$ system that are saturated by contributions near threshold. In fact, there is no much hope for improving our results: next order approximation seems to be too complicated for analytical treatment within the regular perturbation theory for NRQCD. The analysis showed a remarkable stability with respect to the next-to-leading one supplied with an optimization procedure in a variational spirit. Having in mind the considerable technical difficulty of computing next approximation and recognizing the necessity of improving the theoretical predictions in view of new high quality experimental data we think that the next step in the near future will be connected with optimization of the present approximation.

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