The Vacuum Polarization Function to $O(\alpha^2)$ Accuracy
Near Threshold and Darwin Corrections

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Abstract

The QED vacuum polarization function is calculated to $O(\alpha^2)$ (next-to-leading order) accuracy in the threshold regime by using the concept of effective field theories to resum diagrams with the instantaneous Coulomb exchange of longitudinally polarized photons. It is shown that the $O(\alpha^2)$ contributions are of order $\alpha^2$ in size rather than $\alpha^2/\pi^2$. The vacuum polarization contributions to the $O(\alpha^6)$ hyperfine splitting of the positronium ground state are recalculated and differences with an older calculation are pointed out. The results are used to determine $O(C_F^2\alpha_s^4)$ (next-to-next-to-leading order) Darwin corrections to heavy quark-antiquark bound state $l = 0$ wave functions at the origin and to the heavy quark-antiquark production cross section in $e^+e^-$ collisions in the threshold region. The absolute value of the corrections amounts to $10\% - 20\%$ and $17\% - 34\%$ in the modulus squared of the ground state wave functions at the origin for the $b\bar{b}$ and $c\bar{c}$ systems, respectively. In the case of the $tt$ production cross section in the threshold region the absolute value of the corrections is between $2\%$ and $6\%$ around the $1S$ peak and between $1\%$ and $2\%$ for higher energies. A critical comment on recent QCD sum rule calculations for the $\Upsilon$ system is made.
1 Introduction

In recent years many sophisticated methods have been developed to calculate higher order (“multi-loop”) QCD radiative corrections for high energy quantities for which it is believed that an expansion in terms of Feynman diagrams with a certain number of loops represents an excellent approximation to the predictions of quantum chromodynamics. Notable examples are the hadronic cross section in $e^+e^-$ collisions at LEP energies or the (photonic) vacuum polarization function. In the high energy limit, where the quarks can be treated as massless, these quantities have been calculated up to three loops \[1, 2, 3, 4\]. However, future experiments (NLC, B-factory and τ-charm factory) will test the vacuum polarization function and the hadronic cross section also in the kinematic regime close to heavy quark-antiquark thresholds, where bound state effects become important. The threshold regime is characterized by the relation

$$|\beta| \lesssim \alpha_s, \quad \beta \equiv \sqrt{1 - \frac{4 M_Q^2}{q^2 + i\epsilon}},$$

(1)

where $M_Q$ is the heavy quark mass and $\sqrt{q^2}$ denotes the c.m. energy. In the process of heavy quark-antiquark production above threshold, $q^2 > 4M_Q^2$, $\beta$ is equal to the velocity of the quarks in the c.m. frame. We therefore call $\beta$ “velocity” in the remainder of this work, even if $q^2 < 4M_Q^2$. In the threshold regime the accuracy of theoretical predictions to the hadronic cross section and to the vacuum polarization function is much poorer than for high energies. Aside from definitely non-perturbative effects (in the sense of “not calculable from first principles in QCD”), the breakdown of the perturbative expansion in the number of loops makes any theoretical description in the threshold region difficult. This breakdown of the perturbation series is indicated by power $(1/\beta)$ or logarithmic $(\ln \beta)$ divergences in the velocity which blow up if evaluated very close to the threshold point. Some of these divergences (e.g. the $\alpha^n/\beta^n, n > 1$, Coulomb singularities in the Dirac form factor $F_1$ describing the electromagnetic vertex) can be treated by using well-known results from non-relativistic quantum mechanics, but a systematic way to calculate higher-order corrections in the threshold regime seems to be far from obvious, at least from the point of view of covariant perturbation theory in the number of loops. This type of perturbation theory will be referred to as “conventional perturbation theory” from now on in this work.

On the other hand, there are many examples of heavy quark-antiquark bound state properties where the complete knowledge of higher-order corrections would be extremely valuable. Most of the present analyses (see e.g. \[5\]) are based on leading and next-to-leading order calculations. Here, higher-order corrections could significantly increase the precision of present theoretical calculations, but could also serve as an instrument to test how trustworthy certain theoretical predictions are and to estimate the size of theoretical uncertainties. Further, they could contribute toward a better understanding of the role of non-perturbative effects (in the sense mentioned above) in apparent discrepancies between the determination of the size of the strong coupling from the $\Upsilon(1S)$ decay rates \[6\] and QCD sum rule calculations for the $\Upsilon$ system \[7\] on the one hand, and from the LEP experiments on the other.

The framework in which bound state properties and also dynamical quantities in the threshold regime can be calculated in a systematic way to arbitrary precision is non-relativistic quantum chro-

\[1\] During completion of this paper we became aware of a new publication, where QCD sum rules for the $\Upsilon$ system are used to determine the strong coupling and the bottom quark mass \[8\]. We will give a brief comment on this publication and on \[7\] at the end of Section 5.
modynamics (NRQCD) which is based on the concept of effective field theories. In the kinematic regime where bound states occur and slightly above the threshold, NRQCD is superior to conventional perturbation theory in QCD and (at least from the practical point of view) also to the Bethe-Salpeter approach, because it allows for an easy and transparent separation of long- and short-distance physics contributions. This is much more difficult and cumbersome with the former two methods. However, we would like to emphasize that all methods lead to the same results. As an effective field theory, NRQCD needs the input from short-distance QCD in order to produce viable predictions in accordance with quantum chromodynamics. This adjustment of NRQCD to QCD is called the matching procedure and generally requires multi-loop calculations in the framework of conventional perturbation theory at the level of the intended accuracy.

In this work we demonstrate the efficient use of the concept of effective field theories to calculate the QED vacuum polarization function in the threshold region to $\mathcal{O}(\alpha^2)$ accuracy. In order to convince the reader of the simplicity of the approach we use our result to recalculate the vacuum polarization contributions to the $\mathcal{O}(\alpha^6)$ hyperfine splitting of the positronium ground state energy level without referring back to the Bethe-Salpeter equation. Differences between our result and an older calculation [9, 10], are pointed out. We analyse the vacuum polarization function at the bound state energies and above threshold and, in particular, concentrate on the size of the $\mathcal{O}(\alpha^2)$ corrections. It is shown that the size of the $\mathcal{O}(\alpha^2)$ corrections in the threshold regime is of order $\alpha^2$ rather than $\alpha^2/\pi^2$ which is a consequence of their long-distance origin. In a second step our results for the QED vacuum polarization function are applied to calculate $\mathcal{O}(C_F^2\alpha_s^2)$ (next-to-next-to-leading order) Darwin corrections to the heavy quark-antiquark $l = 0$ bound state wave functions at the origin and to the cross section of heavy quark-antiquark production in $e^+e^-$ annihilation (via a virtual photon) in the threshold region. The corresponding unperturbed quantities are the solutions of the Schrödinger equation for a stable quark-antiquark pair with a Coulomb-like QCD potential, $V_{QCD}(r) = -C_F\alpha_s/r$. It is demonstrated that the size of the $\mathcal{O}(C_F^2\alpha_s^2)$ Darwin corrections is also of order $\alpha_s^2$ rather than $\alpha_s^2/\pi^2$. We present simple physical arguments that the scale of the strong coupling governing the $\mathcal{O}(C_F^2\alpha_s^2)$ Darwin corrections is of order $C_F M_Q\alpha_s$ and we analyze the size of the corrections for the $t\bar{t}$, $b\bar{b}$ and $c\bar{c}$ systems assuming that the size of the Darwin corrections can be taken as an order of magnitude estimate for all (yet unknown) $\mathcal{O}(\alpha_s^2)$ corrections. The sign of the latter corrections and their actual numerical values can, of course, only be determined by an explicit calculation of all $\mathcal{O}(\alpha_s^2)$ contributions. At this point we want to emphasize that our approach does not depend on any model-like assumptions, but represents a first principles QCD calculation. The only assumptions (for heavy quarks) are that (i) the instantaneous (i.e. uncrossed) Coulomb-like exchange of longitudinal gluons (in Coulomb gauge) between the heavy quarks leads to the dominant contributions in the threshold regime and is the main reason for heavy quark-antiquark bound state formation and that (ii) all further interactions can be treated as a perturbation. We believe that the actual size of the $\mathcal{O}(\alpha_s^2)$ corrections can then serve as an important a posteriori justification or falsification of these assumptions for the different heavy quark-antiquark systems. Finally, we address the question whether bound state effects can lead to large corrections to the vacuum polarization function in kinematical regions far from the actual threshold regime. We come to the conclusion that such corrections do not exist.

The program for this work is organized as follows: In Section 2 the calculation of the QED vacuum polarization function to $\mathcal{O}(\alpha^2)$ accuracy in the threshold region is presented. We define a renormalized version of the Coulomb Green function for zero distances, which allows for application
of (textbook quantum mechanics) time-independent perturbation theory to determine higher-order corrections to wave functions and energy levels. For completeness we also give an expression for the QED vacuum polarization function valid for all energies with $\mathcal{O}(\alpha^2)$ accuracy. In Section 3 the QED vacuum polarization function in the threshold region is analysed with special emphasis on the size of the $\mathcal{O}(\alpha^2)$ corrections, and the $\mathcal{O}(\alpha^6)$ vacuum polarization contributions to the positronium ground state hyperfine splitting are calculated. Section 4 is devoted to the determination and analysis of the $\mathcal{O}(G_F^2\alpha^2)$ Darwin corrections to the bound state wave functions at the origin and the production cross section in the threshold regime for the different heavy quark-antiquark systems. In Section 5 we comment on the existence of threshold effects far from threshold and Section 6 contains a summary.

2 Determination of the QED Vacuum Polarization Function in the Threshold Region

We consider the QED vacuum polarization function $\Pi$ defined through the one-particle-irreducible current-current correlator

$$
(q^2 g^{\mu\nu} - q^\mu q^\nu) \Pi(q^2) \equiv -i \int d^4x e^{i q x} \langle 0 | T j^\mu(x) j^\nu(0) | 0 \rangle ,
$$

(2)

where $j^\mu(x) = ie \bar{\Psi}(x) \gamma^\mu \Psi(x)$ denotes the electromagnetic current. $\Psi$ represents the Dirac field of the electron with charge $e$. According to the standard subtraction procedure, $\Pi$ vanishes for $q^2 = 0$. It has been shown in [11] that in the kinematical region close to the $e^+e^-$ threshold point $q^2 = 4M^2$, where $M$ denotes the electron mass, the current-current correlator $\Pi$ is directly related to the Green function $G^0_E(\vec{x}, \vec{x'})$ of the positronium Schrödinger equation

$$
\left[ -\frac{1}{M} \vec{\nabla}_x^2 - \frac{\alpha}{|\vec{x}|} - E \right] G^0_E(\vec{x}, \vec{x'}) = \delta^{(3)}(\vec{x} - \vec{y}) ,
$$

(3)

where $E$ denotes the energy relative to the threshold point, $E \equiv \sqrt{q^2 - 2M}$, and $\alpha$ is the fine structure constant. Explicit analytic expressions for the Green function have been calculated in a number of classical papers [12]. The proper relation between the vacuum polarization function and the Green function in the threshold region reads [11]

$$
\Pi^{0,\mathcal{O}(\alpha^2)}_{\text{thr}}(q^2) = \frac{8 \alpha \pi}{q^2} G^0_E(0,0).
$$

(4)

Because we are only interested in $\mathcal{O}(\alpha^2)$ accuracy in the threshold region we effectively can replace the factor $1/q^2$ in eq. (4) by $1/4M^2$.

For illustration, let us now examine the one- and two-loop contributions to the vacuum polarization function and the expression for the vacuum polarization function from non-relativistic quantum mechanics according to eq. (4). The one- and two-loop contributions to $\Pi$ have been known for quite a long time for all energy and mass assignments [13, 14, 15]. Far from the threshold point those loop results provide an excellent approximation to the QED vacuum polarization function at the $\mathcal{O}(\alpha^2)$ accuracy level,

$$
\Pi^{\text{loop}}_{\text{QED}}(q^2) = \left( \frac{\alpha}{\pi} \right) \Pi^{(1)}(q^2) + \left( \frac{\alpha}{\pi} \right)^2 \Pi^{(2)}(q^2) + \mathcal{O}\left( \left( \frac{\alpha}{\pi} \right)^3 \right).
$$

(5)
In the kinematic domain where $\alpha \ll |\beta| \ll 1$, the expansion in terms of the number of loops is still an adequate approximation, and we are allowed to expand the coefficients in eq. (5) for small velocities, 

$$\left(\frac{\alpha}{\pi}\right)^{(1)}(\varphi^2) \mid_{|\beta| \to 0} = \alpha \left[ \frac{8}{9\pi} + \frac{i}{2} \beta \right] + O(\alpha \beta^2),$$

(6)

$$\left(\frac{\alpha}{\pi}\right)^{(2)}(\varphi^2) \mid_{|\beta| \to 0} = \alpha^2 \left[ \frac{1}{4\pi^2} \left( 3 - \frac{21}{2} \zeta_3 \right) + \frac{11}{32} - \frac{3}{4} \ln 2 - \frac{1}{2} \ln(-i \beta) \right] + O(\alpha^2 \beta),$$

(7)

where $\beta = \sqrt{1 - 4M^2/(q^2 + i\epsilon)}$ and $\zeta_3 = 1.202056903\ldots$. In eq. (6) the $O(\alpha \beta)$ contribution is also displayed, allowing for a check of the normalization during the matching procedure. Whereas the one-loop contribution, eq. (6), can be evaluated for $\beta \to 0$, indicating that the $O(\alpha)$ contribution of the vacuum polarization function is of pure short-distance origin, the two-loop expression, eq. (7), diverges logarithmically for vanishing $\beta$. This shows that beyond $O(\alpha)$ accuracy conventional perturbation theory is inadequate for $|\beta| \lesssim \alpha$ due to long-distance effects which cannot be calculated in terms of a finite number of loop diagrams. These long-distance effects can, on the other hand, be described adequately by the vacuum polarization function calculated in the framework of quantum mechanics, which *per constructionem* is valid in the non-relativistic limit. However, the vacuum polarization function as defined in eq. (4) gives a divergent result.\(^2\)

$$\Pi_{Thr}^{0,\mathcal{O}(\alpha^2)}(\varphi^2) = \frac{2\alpha \pi}{M^2} \lim_{r \to 0} G_E^0(0, r)$$

$$= \frac{2\alpha \pi}{M^2} \lim_{r \to 0} \left[ -i \frac{M^2 \beta}{2\pi} e^{M\beta r} \int_0^\infty e^{2iM\beta r t} \left( \frac{1 + t}{t} \right)^{\frac{\alpha}{2\beta}} dt \right]$$

$$= \alpha \left[ \frac{1}{2M r} + \frac{i}{\beta^2} \right] + \alpha^2 \left[ \frac{1}{2} - \gamma - \frac{1}{2} \ln(-2iM\beta r) - \frac{1}{2} \Psi \left( 1 - \frac{i}{2\beta} \right) \right],$$

(8)

where $\gamma$ is the Euler constant and $\Psi$ represents the digamma function,

$$\gamma = \lim_{n \to \infty} \left[ -\ln n + \sum_{i=1}^n \frac{1}{i} \right] = 0.5772156649\ldots,$$

$$\Psi(z) = \frac{d}{dz} \ln \Gamma(z).$$

The divergences in eq. (8) can be easily understood if non-relativistic quantum mechanics is considered as a low-energy effective theory which is capable of describing long-distance physics close to the threshold (characterized by momenta below the scale of the electron mass) but does not know *per se* any short-distance effects coming from momenta beyond the scale of the electron mass. This lack of information is indicated in eq. (8) by short distance (UV) divergences and has to be cured by matching non-relativistic quantum mechanics to QED. The result of this matching procedure is called “non-relativistic quantum electrodynamics” (NRQED) \cite{NRQED}. In this light we have to regard relations (4) and (8) as unrenormalized, which we have indicated by using the superscripts 0.

In the common approach the Lagrangian of NRQED is obtained by introducing higher dimensional operators in accordance with the underlying symmetries of the theory and by matching them to

\(^2\) In eq. (8) we can identify $\beta = \sqrt{1 - 4M^2/(q^2 + i\epsilon)}$ with $\sqrt{(E + i\epsilon)/M}$ because we are interested in $\mathcal{O}(\alpha^2)$ accuracy only.
predictions within conventional perturbation theory in QED in the kinematical regime $\alpha \ll |\beta| \ll 1$ where both NRQED and QED are valid and must give the same results. In general this leads to divergent renormalization constants multiplying the NRQED operators which then cancel the divergences in eq. (8) and add the correct finite short-distance contributions. In our case, however, the explicit determination of the renormalization constants is not necessary because we can match the vacuum polarization function obtained from unrenormalized NRQED directly to the one- and two-loop expressions from QED, eqs. (6) and (7). This “direct matching” method has the advantage that the regularization of the UV divergences in eq. (8) can be performed in a quite sloppy way, but has the disadvantage that it is of no value to determine other quantities than the vacuum polarization function itself. To arrive at the vacuum polarization function in the threshold region we just have to replace the $\beta$-independent and divergent contributions of the $O(\alpha)$ and $O(\alpha^2)$ coefficients of expression (8) in an expansion for small $\alpha$

$$\Pi^{0,\mathcal{O}(\alpha^2)}_{\text{Thr}}(q^2) = \alpha \left[ \frac{1}{2M} + \frac{i}{2} \beta \right] + \alpha^2 \left[ \frac{1}{2} - \frac{1}{2} \gamma - \frac{1}{2} \ln(-2iMr\beta) \right] + A(\alpha, \beta),$$

(9)

$$A(\alpha, \beta) \equiv -\frac{\alpha^2}{2} \left[ \gamma + \Psi \left( 1 - \frac{i}{2} \frac{\alpha}{\beta} \right) \right]$$

(10)

by the corresponding $\beta$-independent and finite contributions in eqs. (6), (7). The correct normalization between the contributions coming from the loop calculations and from non-relativistic quantum mechanics can be checked explicitly by observing that the coefficients in front of the $\beta$-dependent $O(\alpha)$ and $O(\alpha^2)$ contributions in eqs. (6), (7) and (9) are identical. At this point we would like to note that the function $A$ contains only contributions of order $\alpha^3$ and higher for an expansion in small $\alpha$. We shall return to this point later. The final result for the vacuum polarization function valid to $O(\alpha^2)$ accuracy in the threshold region then reads

$$\Pi^{\mathcal{O}(\alpha^2)}_{\text{Thr}}(q^2) = \alpha \left[ \frac{8}{9\pi} + \frac{i}{2} \beta \right] + \alpha^2 \left[ \frac{1}{4\pi^2} \left( 3 - \frac{21}{2} \zeta_3 \right) + \frac{11}{32} - \frac{3}{4} \ln 2 - \frac{1}{2} \ln(-i\beta) \right] + A(\alpha, \beta).$$

(11)

It is an interesting fact that this result can be obtained directly from the one- and two-loop results, eqs. (6) and (7), by the replacement

$$\ln(-i\beta) \rightarrow H(\alpha, \beta) \equiv \gamma + \ln(-i\beta) + \Psi \left( 1 - \frac{i}{2} \frac{\alpha}{\beta} \right) = \ln(-i\beta) - \frac{2}{\alpha^2} A(\alpha, \beta).$$

(12)

As mentioned earlier, the function $A$ is of order $\alpha^3$ for $\alpha \ll |\beta|$. In the language of Feynman diagrams $A$ arises from diagrams with instantaneous Coulomb exchange of two and more longitudinal photons

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3 For $\alpha \ll |\beta| \ll 1$ conventional perturbation theory in QED is valid because $\alpha$ represents the smallest parameter, whereas NRQED is valid because $|\beta|$ is much smaller than the speed of light.
(in Coulomb gauge) between the electron-positron pair. However, if $|\beta|$ is smaller than $\alpha$ ($\beta$ being real), then $A$ is of order $\alpha^2$,

$$A(\alpha, \beta) \overset{|\beta| \ll \alpha}{=} \frac{\alpha^2}{2} \left[ \ln \left( i \frac{2\beta}{\alpha} \right) - \gamma \right] + \mathcal{O}(\alpha \beta).$$

At this point it is illustrative to examine the limits $\alpha \ll \beta$ and $\beta \ll \alpha$ for the function $H$, defined in eq. (12), for real and positive values of $\beta$:

$$H(\alpha, \beta) \overset{\alpha \ll \beta}{=} \ln(-i \beta) + \mathcal{O}\left( \frac{\alpha}{\beta} \right),$$

$$H(\alpha, \beta) \overset{\beta \ll \alpha}{=} \ln\left( \frac{\alpha}{2} \right) + \gamma - i \pi + \mathcal{O}\left( \frac{\beta}{\alpha} \right).$$

It is evident that the function $H$ interpolates between a $\ln \beta$-behaviour in the region where conventional perturbation theory is valid and a constant with a logarithm of $\alpha$ for $\beta/\alpha \to 0$. This leads to a finite value for $\Pi_{\text{Thr}}^{\mathcal{O}(\alpha^2)}$ at the threshold point. As we will see in the next section, $\Pi_{\text{Thr}}^{\mathcal{O}(\alpha^2)}$ has singularities at the positronium energy levels indicating that the breakdown of conventional perturbation theory is directly related to the formation of bound states of the virtual $e^+e^-$ pair [11].

Based on result (11) we are now able to define a renormalized expression for the zero-distance Green function by inverting relation (4)

$$G_E^R(0,0) \equiv \frac{M^2}{2\alpha \pi} \Pi_{\text{Thr}}^{\mathcal{O}(\alpha^2)}(q^2),$$

As we will show later, this renormalized zero-distance Green function can be used for the calculation of higher-order corrections in time-independent perturbation theory.

For completeness we also present the QED vacuum polarization function with $\mathcal{O}(\alpha^2)$ accuracy for all energies,

$$\Pi_{\text{QED}}^{\mathcal{O}(\alpha^2)}(q^2) = \left( \frac{\alpha}{\pi} \right) \Pi^{(1)}(q^2) + \left( \frac{\alpha}{\pi} \right)^2 \Pi^{(2)}(q^2) + A(\alpha, \beta)
\begin{align*}
= \left( \frac{\alpha}{\pi} \right) \left\{ \frac{8 - 3\beta^2}{9} + \frac{\beta (3 - 3\beta^2)}{6} \ln(-p) \right\} \\
+ \left( \frac{\alpha}{\pi} \right)^2 \left\{ \frac{18 - 13\beta^2}{24} + \frac{\beta (5 - 3\beta^2)}{8} \ln(-p) - \frac{(1 - \beta) (33 - 39\beta - 17\beta^2 + 7\beta^3)}{96} \ln(-p)^2 \right. \\
\left. + \frac{\beta (-3 + \beta^2)}{3} \left[ 2 \ln(1-p) \ln(-p) + \ln(-p) \ln(1+p) + \Li_2(-p) + 2\Li_2(p) \right] \right. \\
\left. + \frac{(3 - \beta^2)(1 + \beta^2)}{12} \left[ 2 \ln(1-p) \ln(-p)^2 + \ln(-p)^2 \ln(1+p) \right. \\
\left. + 4 \ln(-p) \Li_2(-p) + 8 \ln(-p) \Li_2(p) - 6 \Li_3(-p) - 12 \Li_3(p) - 3 \zeta_3 \right] \right\} \\
+ A(\alpha, \beta),
\end{align*}$$

where

$$p \equiv \frac{1 - \beta}{1 + \beta}.$$
and \( \text{Li}_2 \), \( \text{Li}_3 \) denote the di- and trilogarithms \([17]\). The reader should note that \( \Pi^{\text{O}(\alpha^2)}_{\text{QED}} \) vanishes at \( q^2 = 0 \) and is an analytic function in \( q^2 \) except at poles and branch cuts, and satisfies the dispersion relation

\[
\Pi^{\text{O}(\alpha^2)}_{\text{QED}}(q^2) = \frac{q^2}{\pi} \int_{-\infty}^{\infty} \frac{dq'^2}{q'^2} \frac{1}{q'^2 - q^2 - i \epsilon} \text{Im}\Pi^{\text{O}(\alpha^2)}_{\text{QED}}(q'^2).
\]

(18)

The explicit form of \( \text{Im}\Pi^{\text{O}(\alpha^2)}_{\text{QED}} \) in the threshold region will be presented in Section 3. For the use and interpretation of formula (17) see also Section 5.

3 Examination of the Vacuum Polarization Function in the Threshold Region

In this section we analyse the properties of the vacuum polarization function in the threshold region above and below the threshold point \( q^2 = 4M^2 \). Compared to an older work on the same subject \([11]\) we are not so much interested in general properties of perturbation theory in the presence of bound state formation, but in the explicit form and behaviour of \( \Pi^{\text{O}(\alpha^2)}_{\text{Thr}} \). In particular, we focus on the size of the \( \mathcal{O}(\alpha^2) \) contributions. We also would like to mention that the vacuum polarization function has been studied in a similar way in \([3]\). In the latter publication, however, a different definition for the vacuum polarization is employed, only the positronium ground state energy is considered and a contribution in the one-loop result is missing. We will come back to this point later. Comparing the methods used in \([3]\) with the effective field theoretical approach employed in this work makes the elegance of the latter technique obvious.

We start in the kinematic region above threshold where \( \alpha \ll \beta \ll 1 \). Here, as mentioned in the previous section, the one- and two-loop results, eqs. (5)-(7), are reliable. This is consistent with the fact that the function \( A \) contains only contributions of order \( \alpha^2 \) and higher,

\[
A(\alpha, \beta) \approx \frac{\alpha^2}{2} \sum_{n=2}^{\infty} \zeta_n \left( i \frac{\alpha}{2 \beta} \right)^{n-1} = \alpha^3 \left[ \frac{i \pi^2}{24 \beta} \right] - \alpha^4 \left[ \frac{\zeta_3}{8 \beta^2} \right] + \mathcal{O}(\frac{\alpha^5}{\beta^3}).
\]

(19)

Thus, for practical applications the contributions of function \( A \) can be neglected. (See also the discussion in Section 3.) One might think that for \( \alpha \approx \beta \) the one- and two-loop expressions should still represent an appropriate \( \mathcal{O}(\alpha^2) \) prediction, because the radius of convergence of the series on the r.h.s. of eq. (19) is \( |\beta| = \alpha/2 \) \([18]\). However, as illustrated in Fig. 1, for \( \alpha \approx \beta \) the contributions coming from function \( A \) are already of order \( \alpha^2/\pi^2 \) and thus have to be included if \( \mathcal{O}(\alpha^2) \) accuracy is intended. For even smaller velocities, of course, the contributions from \( A \) are essential because they cancel the divergent \( \ln \beta \) term from the two-loop expression \( \Pi^{(2)} \), see eqs. (7) and (13). Therefore the value of \( \Pi^{\text{O}(\alpha^2)}_{\text{Thr}} \) at the threshold point is finite and reads \([4]\) (\( \alpha = 1/137 \))

\[
\Pi^{\text{O}(\alpha^2)}_{\text{Thr}}(q^2) = \left[ \frac{\alpha^3}{24 \beta} \right] - \alpha^4 \left[ \frac{\zeta_3}{8 \beta^2} \right] + \mathcal{O}(\frac{\alpha^5}{\beta^3}).
\]

(20)

\( \Pi^{\text{O}(\alpha^2)}_{\text{Thr}} \) indicates that the expression on the r.h.s. of eq. (20) represents only a right-sided limit on the real \( q^2 \)-axis.
Figure 1: The $O(\alpha^2)$ corrections to the vacuum polarization function in the threshold region with and without the contributions contained in function $A$, eq. (11), in the kinematic region $0 < \beta < 2\alpha$ above the threshold. The solid line denotes $\text{Re}[\Pi^{(2)} + \pi^2/\alpha^2 A]$, the dashed line $\text{Re}\Pi^{(2)}$, the dashed-dotted line $\text{Im}[\Pi^{(2)} + \pi^2/\alpha^2 A]$ and the dotted line $\text{Im}\Pi^{(2)}$. The value of the fine structure constant is taken as $\alpha = 1/137$. $\Pi^{(2)}$ represents the two-loop contribution to the vacuum polarization function and is displayed for in eq. (9).

\[ \Pi^{O(\alpha^2)}_{\text{Thr}}(q^2 \to 4M^2+) = \left( \frac{\alpha}{\pi} \right)^8 + \alpha^2 \left[ -\frac{1}{2} \ln \alpha - \frac{1}{2} \gamma + \frac{1}{4} \pi^2 \left( 3 - \frac{21}{2} \zeta_3 \right) + \frac{11}{32} - \frac{1}{4} \ln 2 + i \frac{\pi}{2} \right] \]
\[ = 0.89 \left( \frac{\alpha}{\pi} \right) + \left( -0.36 - \frac{1}{2} \ln \alpha + i \frac{\pi}{2} \right) \alpha^2 = 0.89 \left( \frac{\alpha}{\pi} \right) + \left( 2.10 + i \frac{\pi}{2} \right) \alpha^2. \quad (20) \]

It is evident from eq. (20) and Fig. 1 that the size of the $O(\alpha^2)$ corrections in the threshold region is of order $\alpha^2$ rather than $\alpha^2/\pi^2$, whereas the $O(\alpha)$ contribution is of order $\alpha/\pi$. This can be understood from the fact that the $O(\alpha)$ contribution in $\Pi^{O(\alpha^2)}_{\text{Thr}}$ comes entirely from the one-loop result $\Pi^{(1)}$, eq. (9), and therefore originates from momenta beyond the scale of the electron mass. High momentum contributions are expected to be of order $\alpha/\pi$ if no “large logarithms” occur. The large $O(\alpha^2)$ contributions to $\Pi^{O(\alpha^2)}_{\text{Thr}}$, on the other hand, arise from the interplay of the logarithm of the velocity in $\Pi^{(2)}$, eq. (8), and the contributions from the instantaneous Coulomb-exchange of two and more longitudinal photons between the virtual electron-positron pair. For small velocities the latter effects generate a logarithm of the velocity with an opposite sign, which cancels the logarithm in $\Pi^{(2)}$. We

\footnote{For comparison the reader might consider the well-known one- and two-loop contributions to the anomalous magnetic moment of the electron \[ g_e - 2 = (\frac{\alpha}{\pi}) - 0.66 (\frac{\alpha}{\pi})^2 + O((\frac{\alpha}{\pi})^3). \] Here, long-distance effects from the $e^+e^-$ threshold play no role. Therefore $g_e - 2$ can be regarded as a typical short-distance quantity with no “large logarithms”.}
therefore conclude that the large $\mathcal{O}(\alpha^2)$ contributions are of long-distance origin. This is particularly obvious for the $\ln \alpha$ term which could never be generated at short distances.

The situation for $\alpha \ll |\beta| \ll 1$ below threshold is similar to the one above threshold. Here, the one- and two-loop contributions from conventional perturbation theory, eqs. (5)-(7), provide a viable prediction, because the contributions from the function $A$ are of order $\alpha^3$ and higher. They are beyond the intended accuracy and can be neglected. (See also the discussion in Section 5.) On the other hand, it is obvious that the one- and two-loop results are not sufficient for energies close to the positronium bound state energies,

$$\beta = i \frac{\alpha}{2n} \iff E = -\frac{M \alpha^2}{4n^2}, \quad (n = 1, 2, 3, \ldots), \quad (21)$$

because the vacuum polarization function is expected to have poles at those energy values. Therefore the full expression for $\Pi^{\mathcal{O}(\alpha^2)}_{Thr}$, eq. (11), must be employed. It is straightforward to check that $\Pi^{\mathcal{O}(\alpha^2)}_{Thr}$ indeed has poles at the positronium energy levels $\Pi^0$ leading to the following Laurent expansion at the bound state energies $E_n = -\frac{M\alpha^2}{4n^2}, \ (n = 1, 2, 3, \ldots)$,

$$\lim_{E \to E_n} \Pi^{\mathcal{O}(\alpha^2)}_{Thr}(q^2) = \frac{M \alpha^4}{4n^3} \frac{1}{E_n - E - i\epsilon} + \left(\frac{\alpha}{\pi}\right)^8 + \alpha^2 \left[ a_n \right] + \mathcal{O}(E_n - E), \quad (22)$$

where

$$a_n \equiv -\frac{1}{2} \ln \alpha + \frac{1}{2} \left[ \frac{1}{n} + \ln n - \sum_{i=1}^{n-1} \frac{1}{i} \right] + \frac{1}{4\pi^2} \left( 3 - \frac{21}{2} \zeta_3 \right) + \frac{11}{32} - \frac{1}{4} \ln 2. \quad (23)$$

For completeness we also present the corresponding Laurent expansion for the renormalized zero-distance Green function based on definition (16),

$$\lim_{E \to E_n} G_{E}(0, 0) = \frac{\Psi_n(0)^2}{E_n - E - i\epsilon} + \frac{M^2}{9\pi^2} + \frac{M^2 \alpha}{2\pi} \left[ a_n \right] + \mathcal{O}(E_n - E). \quad (24)$$

As expected, the residues at the bound state energies are equal to the moduli squared of the normalized $l = 0$ Coulomb wave functions at the origin,

$$|\Psi_n(0)|^2 = \frac{M^3\alpha^3}{8\pi n^3}. \quad (25)$$

In eqs. (23)-(24) we have also displayed the constant terms of the Laurent expansion. These constants are relevant for higher-order corrections to the positronium energy levels and to the wave functions at the origin. The size of the $\mathcal{O}(\alpha^2)$ corrections in these constant terms is (similar to the $\mathcal{O}(\alpha^2)$ contributions above threshold) of order $\alpha^2$ rather than $\alpha^2/\pi^2$ indicating again the long-distance character of the $\mathcal{O}(\alpha^2)$ corrections. In Table 1 we have displayed the numerical values of $a_n$ for the radial quantum numbers $n = 1, 2, 3, 4, 5$. It is an interesting fact that the $n \to \infty$ limit of $a_n$ exists

$$\lim_{n \to \infty} \alpha^2 \left[ a_n \right] = \alpha^2 \left[ -\frac{1}{2} \ln \alpha - \frac{1}{2} \gamma + \frac{1}{4\pi^2} \left( 3 - \frac{21}{2} \zeta_3 \right) + \frac{11}{32} - \frac{1}{4} \ln 2 \right] \quad (26)$$

and coincides with $\mathcal{O}(\alpha^2)$ contributions of $\text{Re} \Pi^{\mathcal{O}(\alpha^2)}_{Thr}(q^2 \to 4M^2^+)$, eq. (20). The numerical value for $\lim_{n \to \infty} a_n$ is presented in Table 1.

To illustrate the importance of the constants $a_n$ in time-independent perturbation theory (TIPT), we recalculate the $\mathcal{O}(\alpha^6)$ “vacuum polarization” contributions to the ground state triplet-singlet hyperfine splitting (HFS) of the positronium, which were, to our knowledge, considered for
Table 1: The numerical value for the constants $a_n$ for the radial quantum numbers $n = 1, 2, 3, 4, 5$ and for $n \to \infty$ with $\alpha = 1/137$.

| $n$ | 1   | 2   | 3   | 4   | 5 | $\infty$ |
|-----|-----|-----|-----|-----|---|--------|
| $a_n$ | 2.89 | 2.48 | 2.35 | 2.29 | 2.25 | 2.10 |

the first time in [9]. The vacuum polarization contributions to the HFS in the energy levels of the positronium system arise from the effect that the bound triplet ($^3S_1$, $J^{PC} = 1^{--}$) $e^+e^-$ pair can annihilate into a virtual photon for a time period of order $1/M$, whereas the singlet ($^1S_0$, $J^{PC} = 0^{-+}$) cannot. If the virtual photon energy is approximated by $\sqrt{q^2} = 2M$, this annihilation process leads to a $\delta$-function kernel in the coordinate-space representation (corresponding to a constant kernel in momentum space) with the form,

$$H_{Ann}(\vec{x}) = \frac{2\alpha \pi}{M^2} \delta^{(3)}(\vec{x}).$$  

(27)

This kernel can now be used in TIPT. Taking into account that $\Pi_{Thr}^{\cal O(\alpha^2)}$ contains $\cal O(\alpha)$ as well as $\cal O(\alpha^2)$ contributions we have to apply second- and third-order TIPT to obtain all relevant $\cal O(\alpha^6)$ contributions to the HFS. The formal result for the $\cal O(\alpha^6)$ energy shift for the triplet states with radial quantum numbers $n$ and with $l = 0$ due to $H_{Ann}$ reads

$$\delta E_{Ann,n}^{\alpha^6} = \left\{ \sum_{l \neq n} \langle n | H_{Ann} | l \rangle \frac{|l\rangle \langle l|}{E_n - E_l} H_{Ann} | n \rangle \right\}_{\cal O(\alpha^6)} + \sum_{m \neq n} \sum_{k \neq n} \langle n | H_{Ann} | m \rangle \frac{|m\rangle \langle m|}{E_n - E_m} H_{Ann} | k \rangle \frac{|k\rangle \langle k|}{E_n - E_k} H_{Ann} | n \rangle \right\}_{\cal O(\alpha^6)},$$

(28)

where $|i\rangle$, $i = l, m, n, k$, represent normalized (bound state and free scattering) eigenfunctions to the positronium Schrödinger equation with the eigenvalues $E_i$. The symbol $\left\{ \right\}_{\cal O(\alpha^6)}$ indicates that only $\cal O(\alpha^6)$ contributions are taken into account. It is evident from the form of $H_{Ann}(\vec{x})$ that only the zero-distance Green function is relevant for $\delta E_{Ann,n}^{\alpha^6}$,

$$\sum_{l \neq n} \langle 0 | \frac{|l\rangle \langle l|}{E_l - E_n} | 0 \rangle = \sum_{l \neq n} \frac{|\Psi_l(0)|^2}{E_l - E_n}$$

$$= \lim_{E \to E_n} \left[ G_E^0(0,0) - \frac{|\Psi_n(0)|^2}{E_n - E - i\epsilon} \right].$$

(29)

However, relation (29) still contains divergences (see eq. (8)). As we have pointed out in Section 2, these divergences indicate that non-relativistic quantum mechanics is not capable to describe physics if the relative distance of the electron-positron pair is smaller than the inverse electron mass. Therefore, we have to replace $G_E^0(0,0)$ in relation (29) by its renormalized version $G_E^{\text{R}}(0,0)$, eq. (16) (using eq. (11)), which describes short-distance physics properly. The final expression for $\delta E_{Ann,n}^{\alpha^6}$ then reads

$$\delta E_{Ann,n}^{\alpha^6} = |\Psi_n(0)|^2 \left\{ \left[ \frac{2\alpha \pi}{M^2} \right]^2 \left( -\frac{M^2\alpha}{2\pi} a_n \right) + \left[ \frac{2\alpha \pi}{M^2} \right]^3 \left( -\frac{4}{9} \frac{M^2}{\pi^2} \right)^2 \right\}.$$
\[
\frac{M \alpha^6}{4 \pi^3} \left\{ \frac{1}{2} \ln \alpha - \frac{1}{2} \left( \frac{1}{n} + \ln n - \sum_{i=1}^{n-1} \frac{1}{i} \right) + \frac{1}{4 \pi^2} \left( \frac{13}{81} + \frac{21}{2} \zeta_3 \right) - \frac{11}{32} + \frac{1}{4 \ln 2} \right\}.
\]
(30)

Taking also into account that the virtual photon energy is smaller than \(2M\) by the amount of the binding energy \(E_n = -\frac{M^2}{4\pi^2}\) we have to replace \(M^2\) in eq. (27) by \((M + E_n/2)^2\) and therefore get another \(\mathcal{O}(\alpha^6)\) contribution,

\[
\delta E_{\text{Ann},n}^6 = \frac{\alpha^2}{4n^2} \delta E_{\text{Ann},n}^4 = \frac{M \alpha^6}{16n^5},
\]
(31)

where \(\delta E_{\text{Ann},n}^4\) represents the \(\mathcal{O}(\alpha^4)\) energy shift due to \(H_{\text{Ann}}\). For the ground state \((n = 1)\) the complete \(\mathcal{O}(\alpha^6)\) vacuum polarization contribution to the HFS then reads

\[
\delta E_{\text{Ann},1}^6 + \delta E_{\text{Bind},1}^6 = \frac{M \alpha^6}{4} \left\{ \frac{1}{2} \ln \alpha + \frac{1}{4 \pi^2} \left( \frac{13}{81} + \frac{21}{2} \zeta_3 \right) - \frac{11}{32} + \frac{1}{4 \ln 2} \right\}.
\]
(32)

Our result differs from the one presented in [8, 10] by the amount \(M \alpha^6/8\). Half of the discrepancy comes from the fact that in [8] the binding energy contribution \(\delta E_{\text{Bind},1}^6\) was not taken into account, whereas the other half originates from a missing \(\mathcal{O}(\alpha^2)\) contribution in the one-loop vacuum polarization [10].

Before we turn to applications of our results in the context of QCD, we do not want to leave unmentioned that the leading contributions to the normalized cross section for production of a heavy lepton-antilepton pair (with lepton mass \(M\)) in \(e^+e^-\) collisions (via a virtual photon) in the threshold region can be recovered from \(\Pi_{\text{Thr}}^{\mathcal{O}(\alpha^2)}\) by means of the optical theorem [20, 21],

\[
R_{\text{Thr}}^{L^+L^-} = \frac{\sigma(\gamma^* \rightarrow \gamma^* \rightarrow L^+L^-)}{\sigma_{\text{pt}}} = \frac{3}{\alpha} \text{Im} \Pi_{\text{Thr}}^{\mathcal{O}(\alpha^2)}(q^2) = \frac{6\pi}{M^2} \text{Im} G_E^R(0,0)
\]

\[
= \frac{6\pi^2}{M^2} \sum_{n=1}^{\infty} |\Psi_n(0)|^2 \delta(E - E_n) + \Theta(E) \frac{3}{2} \frac{\alpha}{1 - \exp(-\frac{\alpha}{2})},
\]
(33)

where \(\sigma_{\text{pt}}\) represents the point cross section and only final-state interactions are taken into account.

\section{4 Darwin Corrections in QCD}

In the previous section we have shown that the size of the \(\mathcal{O}(\alpha^2)\) corrections to the QED vacuum polarization function in the threshold region is of order \(\alpha^2\) rather than \(\alpha^2/\pi^2\). Although this fact is important for precision tests of QED\footnote{This can be easily seen by comparing eq. (33) of [8] with eq. (32) in this work for

\[q^2_{n=1} = (2M - M^2/4)^2 \Leftrightarrow \beta_{n=1} = i \frac{\alpha}{2} + \mathcal{O}(\alpha^3).\]

This shows that at bound state energies the one-loop contribution to the vacuum polarization function also contains terms of order \(\alpha^2\).} it does not lead to theoretical concerns about the convergence

\footnote{As far as tests of QED in the \(\tau^+\tau^-\) system in the threshold region are concerned the present experiments do not even reach the \(\mathcal{O}(\alpha)\) (next-to-leading order) accuracy level. This can be easily seen from the fact that the complete threshold region for the \(\tau^+\tau^-\) system, \(|\beta| < \alpha \Leftrightarrow |\sqrt{q^2 - 2m_{\tau}|} \leq m_{\tau}\alpha^2 = 0.1\text{ MeV} \) still lies within the limits on the tau mass itself, \(m_{\tau} = 1777.00^{+0.30}_{-0.27}\text{ MeV} [22]\). Thus only experiments on electron and muon systems can be regarded as precision tests of QED in the threshold regime.}
of the perturbative series because of the smallness of the fine structure constant $\alpha$ and because QED is not asymptotically free.

In the framework of QCD, however, the situation is completely different: the coupling is much larger and even becomes of order one for scales much lower than 1 GeV. Therefore, the fact that the size of the $O(\alpha_s^2)$ (next-to-next-to-leading order) corrections in the threshold region might be of order $\alpha_s^2$ rather than $\alpha_s^2/\pi^2$ is an extremely important theoretical issue because this would lead to corrections of order $1\% - 25\%$ rather than $0.1\% - 2.5\%$ for $\alpha_s = 0.1 - 0.5$. Here, two natural questions arise: what scale should be used in the strong coupling, and for which heavy quark-antiquark systems the $O(\alpha_s^2)$ corrections represent contributions to the asymptotic perturbation series in the convergent regime. These questions will be addressed in the following section.

To be more specific we will calculate the $O(C_F^2\alpha_s^2)$ Darwin corrections to the $(S$-wave, $l = 0)$ wave functions of a bound heavy quark-antiquark pair at the origin and to the heavy quark-antiquark pair production cross section in $e^+e^-$ annihilation (via a virtual photon) in the threshold region. A presentation of all $O(C_F^2\alpha_s^2)$ corrections including all kinematic and relativistic effects will given in a subsequent publication. The corresponding uncorrected quantities are the well-known exact solutions to a pure Coulomb-like non-relativistic quark-antiquark system described by a Schrödinger equation

\[ V_{QCD}(r) = -\frac{C_F}{r}, \]

where $C_F = (N_c^2 - 1)/2N_c = 4/3$.

The Darwin correction is generated in the non-relativistic expansion of the Dirac equation. In the coordinate-space representation it is proportional to a $\delta$-function and reads

\[ H_{Dar}(\vec{x}) = \frac{C_F \alpha_s \pi}{M_Q^2} \delta^{(3)}(\vec{x}). \]

A practical application for the corrections to the bound state wave functions at the origin is the leptonic decay rate of the $J/\Psi$ and the $\Upsilon(1S)$ and (maybe) of the first few excited states of the $\Upsilon$ family, whereas the corrections to the cross section would be relevant for $t\bar{t}$ production at NLC. We explicitly mention those applications in this context because it is believed that for them non-perturbative (in the sense “not calculable from first principles in QCD”) effects are either well under control or even negligible [23, 20]. But, of course, these corrections can be applied to other heavy quark-antiquark systems as well, at least in order to check their size. At this point we want to emphasize that we do not intend to present a thorough phenomenological analysis in this work. The primary aim is to use the $O(C_F^2\alpha_s^2)$ Darwin corrections to illustrate the typical size of the complete (and yet unknown) $O(\alpha_s^2)$ corrections for the $t\bar{t}$, $b\bar{b}$ and $c\bar{c}$ systems. Their actual numerical value and even their sign cannot, of course, be predicted at the present stage.

To keep our analysis transparent we ignore all $O(\alpha_s)$ corrections, the effects from the running of the strong coupling and also non-perturbative contributions like the gluon condensate. The latter effects are well known and have been treated in a large number of earlier publications. We further neglect the width of the quarks and treat them as stable particles for the most part in the following analysis. From the technical point of view the calculations of the $O(C_F^2\alpha_s^2)$ Darwin corrections are identical to the corresponding QED calculations, which means that we use time-independent perturbation theory. However, we have to take care about the correct implementation of the number of colors, $N_c = 3$, and the group theoretical factor $C_F$. In the following the superscript “QCD” indicates that the corresponding quantity is obtained from the QED expression by the replacement $\alpha \rightarrow C_F\alpha$.

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8 Compared to the Darwin interaction known from the hydrogen atom the expression on the r.h.s. of eq. (34) is a factor of two larger because both quark-antiquark-gluon vertices contribute.
It is then straightforward to determine the $\mathcal{O}(C_F^2\alpha_s^2)$ Darwin corrections to the modulus squared of the $l = 0$ bound state wave functions at the origin, $(n = 1, 2, 3, \ldots)$,

$$\delta|\Psi_n^{\text{QCD}}(0)|_{\text{Dar}}^2 = -2|\Psi_n^{\text{QCD}}(0)| \left\{ \frac{C_F\alpha_s\pi}{M_Q^2} \lim_{E \to E_n^{\text{QCD}}} \left[ G_{E,\text{Dar}}^{R,\text{QCD}}(0,0) - \frac{|\Psi_n^{\text{QCD}}(0)|^2}{E_n^{\text{QCD}} - E - i\epsilon} \right] \right\}_{\mathcal{O}(C_F^2\alpha_s^2)}$$

$$= -|\Psi_n^{\text{QCD}}(0)|^2 C_F^2\alpha_s^2 e_n^{\text{QCD}}, (35)$$

where the symbol $\{\_{\mathcal{O}(C_F^2\alpha_s^2)}\}$ indicates that only $\mathcal{O}(C_F^2\alpha_s^2)$ corrections are taken into account\footnote{Eq. (33) also generates $\mathcal{O}(C_F\alpha_s)$ corrections which differ from the well-known $\mathcal{O}(C_F\alpha_s)$ corrections generated by the $(1 - 4C_F\alpha_s/\pi)$ correction factor \cite{24}. Adding up all the $\mathcal{O}(C_F\alpha_s)$ corrections and the corresponding renormalization constants will of course yield the correct result. The same remark holds for the result for the cross section above threshold, eq. (37).}. The calculation of the $\mathcal{O}(C_F^2\alpha_s^2)$ Darwin corrections to the quark-antiquark cross section in the threshold region is more involved. Here, we apply the optical theorem, eq. (33), to the corrections of the zero-distance Green function themselves,

$$\delta G_{E,\text{Dar}}^{R,\text{QCD}}(0,0) = -\frac{C_F\alpha_s\pi}{M_Q^2} \left[ G_{E,\text{Dar}}^{R,\text{QCD}}(0,0) \right]^2. (36)$$

The $\mathcal{O}(C_F^2\alpha_s^2)$ Darwin corrections to the cross section above threshold then read

$$\delta R_{\text{Thr, Dar}}^{QQ} = N_c \frac{6\pi}{M_Q^2} \text{Im}\left[ G_{E,\text{Dar}}^{R,\text{QCD}}(0,0) \right] \left\{ -\frac{2C_F\alpha_s\pi}{M_Q^2} \text{Re}\left[ G_{E,\text{Dar}}^{R,\text{QCD}}(0,0) \right] \right\}_{\mathcal{O}(C_F^2\alpha_s^2, C_F\alpha_s\beta)}$$

$$= R_{\text{Thr}}^{QQ} \left\{ -\text{Re}\Pi_{\text{Thr}}^{\mathcal{O}(C_F^2\alpha_s^2), \text{QCD}}(q^2) \right\}_{\mathcal{O}(C_F^2\alpha_s^2, C_F\alpha_s\beta)}, (37)$$

where $R_{\text{Thr}}^{QQ}$ represents the “Sommerfeld factor” (sometimes also called the “Fermi factor”)

$$R_{\text{Thr}}^{QQ} = N_c \frac{6\pi}{M_Q^2} \text{Im}\left[ G_{E,\text{Dar}}^{R,\text{QCD}}(0,0) \right]$$

$$= N_c \frac{3}{2} \frac{C_F\alpha_s\pi}{1 - \exp(-C_F\alpha_s\pi/\beta)} = N_c \frac{3}{2} \beta \exp\left( \frac{C_F\alpha_s\pi}{2\beta} \right) \Gamma\left( 1 + i \frac{C_F\alpha_s}{2\beta} \right) \Gamma\left( 1 - i \frac{C_F\alpha_s}{2\beta} \right). (38)$$

Below threshold we have to determine the corrections to the residues of $G_{E,\text{Dar}}^{R,\text{QCD}}(0,0)$ at the bound state energies, where as shown above the corresponding bound state poles have to be subtracted. This calculation is straightforward and leads to the corrections to the $l = 0$ bound state wave functions at the origin presented in eq. (35). It is an interesting fact that eq. (37) allows for the calculation of the shifts of the $Q\bar{Q}$ bound state energies due to the Darwin interaction. To show this we rewrite the sum of the Sommerfeld factor, eq. (38), and the contribution involving the digamma function of the $\mathcal{O}(C_F^2\alpha_s^2)$ Darwin corrections above threshold, see eqs. (39), (11) and (37), as

$$R_{\text{Thr}}^{QQ} \left\{ 1 + \frac{C_F^2\alpha_s^2}{4} \left[ \Psi\left( 1 + i \frac{C_F\alpha_s}{2\beta} \right) + \Psi\left( 1 - i \frac{C_F\alpha_s}{2\beta} \right) \right] \right\}$$

$$\rightarrow N_c \frac{3}{2} \beta \exp\left( \frac{C_F\alpha_s\pi}{2\beta} \right) \Gamma\left( \frac{C_F^2\alpha_s^2}{4} + 1 + i \frac{C_F\alpha_s}{2\beta} \right) \Gamma\left( \frac{C_F^2\alpha_s^2}{4} + 1 - i \frac{C_F\alpha_s}{2\beta} \right). (39)$$
It can be easily checked that the function $\Gamma(\frac{C_F^2\alpha_s^2}{4} + 1 - i \frac{C_F\alpha_s}{2\beta})$ develops poles at the energies\(^{10}\)

$$\tilde{E}_n^{QCD} = E_n^{QCD} + \delta E_{n,Dar}^{QCD}, \quad (n = 1, 2, 3, \ldots),$$

where the $\delta E_{n,Dar}^{QCD}$ represent the energy shift of the $l = 0$ Coulomb energy levels with the radial quantum number $n$ generated by the Darwin interaction,

$$\delta E_{n,Dar}^{QCD} = \langle n^{QCD} | H_{Dar} | n^{QCD} \rangle = |\Psi_n^{QCD}(0)|^2 \frac{C_F\alpha_s \pi}{M_Q^2}$$

$$= \frac{M_Q C_F^4 \alpha_s^4}{8 n^3}. \quad (41)$$

At this point we also want to emphasize that the $\ln(C_F\alpha_s)$ and digamma contributions occurring in eqs. (33) and (37) are not related to the running of the strong coupling and therefore cannot be resummed by any known type of renormalization group equation in the sense of a leading logarithmic resummed by any known type of renormalization group equation in the sense of a leading logarithmic resummation. These logarithmic terms arise because two scales are relevant in the threshold region, the heavy quark mass $M_Q$ and the relative momentum of the quark-antiquark pair $\propto C_F\alpha_s M_Q$\(^{25}\). The $\ln(C_F\alpha_s)$ contributions induced by the running of the strong coupling have been discussed in\(^{26, 23}\).

Before we turn to the discussion on the size of the $O(C_F^2\alpha_s^2)$ Darwin corrections we have to address the question of which scale one should use in the strong coupling. Strictly speaking, a final answer to this problem would require an $O(\alpha_s^2)$ analysis, which is beyond the scope of this work. However, one can find simple arguments that the scale in the strong couplings of expressions (33) and (37) should be of the order $C_F\alpha_s M_Q$, which will be called “the soft scale” in the remainder of this work. We would like to remind the reader that the scale of the strong coupling in the unperturbed (pure Coulomb) quantities $|\Psi_n^{QCD}(0)|^2$ and $R_{Thr}^{QCD}$ is of the order of the soft scale. This is obvious for the wave functions of the ground state and the first few excited states and for the cross section in the kinematic region $\beta \approx C_F\alpha_s$ because they describe bound quark-antiquark pairs with relative momentum of order $C_F\alpha_s M_Q$. But it is also true for highly excited states ($n \gg 1$) and the cross section right at the threshold due to “saturation” effects\(^{26, 23}\), i.e. the scale of the strong coupling is of order $C_F\alpha_s M_Q$ although the kinematical relative momentum of the quark pair vanishes\(^{27}\). To understand that the scale of the $O(C_F^2\alpha_s^2)$ Darwin corrections should also be of order of the soft scale, let us have a closer look at the origin of the strong couplings governing these corrections: one power of $\alpha_s$ comes from the Darwin interaction, $H_{Dar}$, and the other power of $\alpha_s$ (including the $\ln(C_F\alpha_s)$ terms) originates from the $O(\alpha_s^2)$ contribution of the vacuum polarization function $\Pi_{Thr}^{QCD}$, $C_F^2\alpha_s^2$. As mentioned in the previous section, the latter contribution is of long-distance origin and therefore governed by the soft scale. In contrast to the pure Coulomb interaction, $1/\vec{p}^2$, the Darwin interaction is a constant in momentum space and consequently sensitive to both low and high momenta. But based on our previous observations of the domination of long-distance effects, we can assume that

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\(^{10}\) It should be noted that the $(1 - 4C_F\alpha_s/\pi)$ correction factor of the cross section is irrelevant for shifts of the bound state energies because the former represents a global multiplicative short-distance factor.

\(^{11}\) In\(^{26, 23}\) a proof for saturation is only given for the cross section above the threshold point. An analogous proof for highly excited states or the cross section slightly below the threshold point does, to our knowledge, not exist in literature. Such a proof is, however, much more difficult due to the breakdown of time-independent perturbation theory for the logarithmic kernel $\delta V(r) \sim \ln(r)/r$ for high radial excitations (see e.g.\(^{23}\)). Nevertheless we find it plausible that saturation also takes place slightly below the threshold point because the cross section at the threshold point $q^2 = 4M_Q^2$ should be well defined.
the scale of the strong coupling in the Darwin interaction should also be the soft scale rather than the heavy quark mass. The size of the strong coupling governing the $O(C_F^2 \alpha_s^2)$ Darwin corrections of eqs. (33) and (34) can therefore be estimated via the self-consistency equation

$$\alpha_s = \alpha_s(C_F \alpha_s M_Q).$$

which leads to $\alpha_s = 0.13 - 0.16$, $0.25 - 0.38$ and $0.34 - 0.59$ for the top, bottom and charm quark systems, respectively. The latter ranges are obtained by using the $\overline{\text{MS}}$ definition for the strong coupling, the one-loop QCD beta-function and $\alpha_s(M_Z = 91.187 \text{GeV}) = 0.125$ and by taking twice and half the argument of the strong coupling on the r.h.s. of relation (42). Further, the mass values in equation (42) have been taken to be the pole values. For the quark (pole) masses we have chosen $M_t = 175 \text{ GeV}$, $M_b = 5 \text{ GeV}$ and $M_c = 1.7 \text{ GeV}$. The reader should note that the prescription given above to calculate the size of the strong coupling is far from being unique. Depending on the choice of the definition of the strong coupling, the quark mass values or the number of loops in the QCD beta-function, larger or smaller values for $\alpha_s$ might result. This dependence on the prescription is particularly strong for the charm system\footnote{As an example, using the two-loop QCD beta-function results in $\alpha_s = 0.13 - 0.17$, $0.27 - 0.44$ and $0.38 - 0.76$ for the top, bottom charm system, respectively. At this point it is clearly obvious that the situation for the charm system is rather hopeless as far as the question of perturbativity is concerned.}. As a consequence the theoretical uncertainties quoted in this work should be more understood as good guesses rather than strict theoretical limits. However, we think that the ranges of the strong coupling given above are good enough in order to illustrate the impact of the $O(C_F^2 \alpha_s^2)$ Darwin corrections in particular for $tt$ production in the threshold region. We also want to emphasize that our conclusions for the perturbativity of the different heavy quark systems do not depend on different prescriptions for the strong coupling.

| $n$ | 1 | 2 | 3 | 4 | $\infty$ |
|-----|---|---|---|---|----------|
| $\Delta_{t\bar{t}}^{\psi,n}$ | $-0.05 / -0.04$ | $-0.04 / -0.03$ | $-0.03 / -0.02$ | $-0.03 / -0.02$ | $-0.02 / -0.02$ |
| $\Delta_{b\bar{b}}^{\psi,n}$ | $-0.20 / -0.11$ | $-0.09 / -0.06$ | $-0.06 / -0.05$ | $-0.05 / -0.04$ | $-0.02 / +0.01$ |
| $\Delta_{c\bar{c}}^{\psi,n}$ | $-0.34 / -0.17$ | $-0.10 / -0.09$ | $-0.06 / -0.01$ | $-0.05 / +0.03$ | $-0.01 / +0.15$ |

Table 2: The relative $O(C_F^2 \alpha_s^2)$ Darwin corrections to the moduli squared of the $l = 0$ bound state wave functions $\Delta_{\psi,n}$ are given for the $t\bar{t}$, $b\bar{b}$ and $c\bar{c}$ system, respectively. Displayed are the smallest and largest values for the range of $\alpha_s$ values given below eq. (12) for the radial quantum numbers $n = 1, 2, 3, 4$ and for $n \to \infty$. In Table 2 the smallest and largest values for the relative $O(C_F^2 \alpha_s^2)$ Darwin corrections to the moduli squared of the $l = 0$ bound state wave functions $\Delta_{\psi,n} \equiv \delta |\Psi_{n}^{\text{QCD}}(0)|^2_{\text{Dar}}/|\Psi_{n}^{\text{QCD}}(0)|^2$ for the different heavy quark systems are displayed for the ground states ($n = 1$) and the first three radial excited states ($n = 2, 3, 4$), employing the ranges for the strong coupling as given below eq. (12). For illustration the corresponding value for ($n \to \infty$) is also presented. The absolute values of the
corrections to the ground states amount to $4\%-5\%$ for the $t\bar{t}$, $11\%-20\%$ for $b\bar{b}$ and $17\%-34\%$ for the $c\bar{c}$ system. It is an interesting fact that for the $b\bar{b}$ and $c\bar{c}$ systems the size of the corrections is rapidly decreasing for higher excited states. In particular, the sensitivity of the corrections to the different values of $\alpha_s$ seems to be surprisingly small for the excited states in the $b\bar{b}$ and $c\bar{c}$ systems. We will come back to this point later.

In Fig. 2a and 3a,b the relative $\mathcal{O}(C_F^2\alpha_s^2)$ Darwin corrections to the (stable) quark-antiquark production cross section $\Delta R_{Q\bar{Q}} \equiv \delta R_{Thr,Dar}^{Q\bar{Q}}/R_{Thr}^{Q\bar{Q}}$ are displayed above the threshold point for the three heavy quark systems in the range $0 < \beta < C_F \alpha_s$. (For $t\bar{t}$ production this corresponds to the energy range $0 < E < 5$ (8) GeV for $\alpha_s = 0.13$ (0.16)) The solid (dashed) lines correspond to the lower (upper) $\alpha_s$ value given below eq. (12). For the $t\bar{t}$ system the size of the relative corrections is quite stable between $-1.9\%$ and $-1.0\%$ with the tendency to decrease in magnitude for larger velocities. It is striking that the dependence of the corrections on the changes in the $\alpha_s$ value is weaker for larger velocities ($0.3\%$ for $\beta = 0$ and $0.05\%$ for $\beta = C_F \alpha_s$). For the $b\bar{b}$ system the corrections vary between $-2\%$ (lower value) and $+5\%$ (upper value) where the larger values occurs for larger velocities. In contrast to the top system the dependence of the corrections on the changes in the $\alpha_s$ value ($3\%$ for
Figure 3: The relative $\mathcal{O}(C_F^2 \alpha_s^2)$ Darwin corrections to the $b\bar{b}$ (a) and $c\bar{c}$ (b) production cross section in the kinematical region $0 < \beta < C_F \alpha_s$ above threshold. The solid line corresponds to $\alpha_s = 0.25$ (0.34) and the dashed line to $\alpha_s = 0.38$ (0.59) for the case of $b\bar{b}$ ($c\bar{c}$) production.

$\beta = 0$ and 5% for $\beta = C_F \alpha_s$) increases for larger velocities. This indicates that the perturbative approach employed in this work works better for the $t\bar{t}$ than for the $b\bar{b}$ system. For the $c\bar{c}$ system, on the other hand, the dependence on the changes in $\alpha_s$ are tremendous. Depending on the size of the coupling the corrections vary from $-1\%$ to $+15\%$ for $\beta = 0$ up to $+3\%$ to $+26\%$ for $\beta = C_F \alpha_s$, drawing a rather uncomfortable picture for the perturbativity in the charm system. For the case of $t\bar{t}$ production we have also plotted the corrections for a finite width $\Gamma_t = 1.5 \text{ GeV}$ (see Fig. 2b) in the energy range $-10 \text{ GeV} < E < +10 \text{ GeV}$ in order to demonstrate the impact of the $\mathcal{O}(C_F^2 \alpha_s^2)$ Darwin corrections in the presence of the large top width. This has been achieved by the naive replacement $E \rightarrow E + i \Gamma_t$ in eqs. (37) and (38). We want to mention that the inclusion of a finite width by this naive procedure does not represent a consistent treatment at the $\mathcal{O}(\alpha_s^2)$ accuracy level. However, we find that this approach is justified here in order to demonstrate that the typical size of the $\mathcal{O}(C_F^2 \alpha_s^2)$ Darwin corrections is not altered if the top quark width is taken into account. In this case the relative $\mathcal{O}(C_F^2 \alpha_s^2)$ Darwin corrections amount to $-6\%$ to $-2\%$ around the $1S$ peak and to $-2\%$ to $-1\%$ for higher energies. For a rigorous treatment of the corrections due to the off-shellness of the top quark we refer the reader to [27] and references therein.
Although the \( \mathcal{O}(C_F^2 \alpha_s^2) \) Darwin corrections discussed above represent only a small part of the full \( \mathcal{O}(\alpha_s^2) \) corrections, we believe that their size can be taken as an order of magnitude estimate for the sum of all \( \mathcal{O}(\alpha_s^2) \) corrections. We therefore have to face the questions whether or how far a perturbative expansion in the strong coupling in the threshold regime makes sense. Because we take the position that one should not automatically reject the possibility of a perturbative treatment of long-distance effects, we think that the \( \mathcal{O}(C_F^2 \alpha_s^2) \) Darwin corrections determined in this work provide us with important hints toward an acceptable answer to this fundamental question from the point of view of perturbation theory itself. There is no doubt that perturbation theory in the strong coupling is still viable for the \( t\bar{t} \) system. It has been shown in [20] by using more general arguments that the large top mass and width serve as a screening device which protects the threshold region from the influence of non-perturbative effects making the \( t\bar{t} \) system into the “hydrogen atom of the strong interaction”. Thus a perturbative treatment of the \( t\bar{t} \) system should exhibit an excellent convergence. This is consistent with the observations from the previous discussions showing that the \( \mathcal{O}(C_F^2 \alpha_s^2) \) Darwin corrections for the top system are at the level of a few percent for the most of the threshold region[13]. This, on the other hand, allows us to conclude that the theoretical uncertainty of all present analyses for the total \( t\bar{t} \) cross section in the threshold region is at the few percent level, because no full \( \mathcal{O}(\alpha_s^2) \) treatment has ever been accomplished there. Further, the theoretical uncertainty of such a complete analysis would then be roughly one to two percent around the 1S peak and below several per mille for higher energies. This can be estimated by taking the \( \alpha_s \) values presented below eq. (42) cubed (assuming that no scales lower than \( C_F \alpha_s M_Q \) are relevant for the corrections beyond the \( \mathcal{O}(\alpha_s^2) \) accuracy level) and by observing the sensitivity of the \( \mathcal{O}(C_F^2 \alpha_s^2) \) Darwin corrections to changes in the values of the strong coupling (see Fig. 2b). To achieve an accuracy much below the percent level at the 1S peak a more rigorous treatment of the scale in the strong coupling governing the \( \mathcal{O}(\alpha_s^2) \) corrections would be needed, i.e. an \( \mathcal{O}(\alpha_s^3) \) calculation.

As far as the \( b\bar{b} \) system is concerned, the situation is worse than for the \( t\bar{t} \) system. It has been shown in a number of classical papers [30, 31, 32] that a proper theoretical description of the bottom system can only be achieved by taking into account non-perturbative corrections, which cannot be calculated from first principles in QCD. On the other hand, it has been demonstrated in [23] that a quite acceptable “parameter-free” description of the \( (S\text{-wave}, l = 0) b\bar{b} \) bound states with low radial excitation is possible by using perturbative calculations supplemented by non-perturbative contributions in the form of the quark or the gluon condensates. However, the latter analyses (as far as corrections to the moduli squared of the wave functions at the origin and to the cross section above threshold are concerned) were essentially based on formulae including only the effects of the one-loop running of the strong coupling and the global \( \mathcal{O}(\alpha_s) \) correction factor \( 1 - 4 C_F \alpha_s/\pi \). The question whether the \( \mathcal{O}(\alpha_s^2) \) perturbative corrections lead to a still converging series was not addressed explicitly. Equipped with the results for the \( \mathcal{O}(C_F^2 \alpha_s^2) \) Darwin corrections, we are able to draw a rough picture concerning the latter question for the case of the moduli squared of the \( l = 0 \) bound state wave functions

\[ \text{A comparison of the size of the } \mathcal{O}(C_F^2 \alpha_s^2) \text{ Darwin corrections with the } \mathcal{O}(C_F \alpha_s) \text{ corrections from the } (1 - 4 C_F \alpha_s/\pi) \text{ suppression factor is slightly misleading in this context because the latter represents a pure short-distance contribution. Therefore the } \mathcal{O}(C_F \alpha_s) \text{ correction should not be included in a discussion on the convergence in the perturbative description of long-distance contributions. However, for the convenience of the reader, the size of the large } \mathcal{O}(C_F \alpha_s) \text{ corrections shall also be given. It has been shown in [1, 23, 24] in a two-loop analysis that the scale in the strong coupling of the } \mathcal{O}(C_F \alpha_s) \text{ suppression factor is } e^{-11/24} M_Q \text{ in the } \overline{\text{MS}} \text{ scheme. This results in } -4 C_F \alpha_s/\pi = -20\%, -41\% \text{ and } -64\% \text{ for the top, bottom and charm systems, respectively, using the one-loop QCD beta-function, the pole mass values given below eq. (42) and } \alpha_s(M_z = 91.187 \text{ GeV}) = 0.125. \]
at the origin. For the ground state the \(O(\alpha_s^2)\) corrections should be between 10% and 20% (where the actual sign of the corrections can only be determined by a complete \(O(\alpha_s^2)\) analysis) with theoretical uncertainties of order \(\pm 5\%\) coming from the ignorance of the actual scale of the strong coupling and other corrections beyond the \(O(\alpha_s^2)\) level. This does not represent an overwhelming convergence, but it is acceptable compared to the precision of experimental measurements\([33]\) and it indicates that an actual determination of all \(O(\alpha_s^2)\) corrections would lead to a considerable improvement of the precision of the theoretical description. It is remarkable that the \(O(C_2\alpha_s^2)\) Darwin corrections seem to indicate that the size of the \(O(\alpha_s^2)\) corrections including their sensitivity to changes in the value of the strong coupling is much smaller for higher excited states (see Table 2). Here, however, non-perturbative contributions get more and more out of control\([31, 32]\) and a complete \(O(\alpha_s^2)\) analysis is therefore necessary to give a trustworthy interpretation of this phenomenon. The latter remark is also true for the \(c\bar{c}\) system.

Finally, we also want to mention the \(c\bar{c}\) system. In view of the \(O(C_2\alpha_s^2)\) Darwin corrections, we can expect the size of the complete \(O(\alpha_s^2)\) corrections to the modulus squared of the ground state wave function at the origin to be at least at the level of 15% to 35% with theoretical errors which might be almost as large as the size of the \(O(\alpha_s^2)\) corrections themselves. (Again we can estimate the size of the corrections beyond the \(O(\alpha_s^2)\) level by taking the long-distance \(\alpha_s\) values given below eq. (42) cubed.) It is evident that in the case of the \(c\bar{c}\) system the limits of perturbation theory are reached or even exceeded. Even with a complete determination of all \(O(\alpha_s^2)\) corrections the theoretical uncertainties would not decrease considerably, which is obviously a consequence of the large size of the strong coupling. We therefore conclude that it will be extremely difficult (if not impossible) to achieve a perturbation theory based theoretical description for the charm system with uncertainties lower than several times 10% if there is no (unforeseen) cancellation among different types of corrections.

To conclude this section there is a remark in order: for the calculations of the \(O(C_2\alpha_s^2)\) Darwin corrections we used the renormalized Green function at zero distances, eq. (16), without any further explanation. This is slightly misleading because it implies that the \(O(C_2\alpha_s^2)\) Darwin corrections to wave functions and cross sections can be uniquely separated from all the other \(O(C_2\alpha_s^2)\) corrections. As far as the \(\ln \alpha_s\) contribution and the digamma term are concerned this is definitely true, but this is not the case for the constant terms. This is a consequence of the divergences which arise during the calculations and which have to be renormalized. The use of our renormalized zero-distance Green function represents one possible way to achieve this renormalization. Nevertheless we think that our approach is justified in order to illustrate the possible size of the complete \(O(\alpha_s^2)\) corrections. This view is also supported by the explicit results for all \(O(C_2\alpha_s^2)\) corrections to the \(l = 0\) wave functions at the origin and the cross section, which will be published shortly. However, we want to emphasize that the latter considerations do not affect the validity of the expressions for the vacuum polarization function presented in Sections 2 and 3. There, all constants are correct due to proper matching to the well established one- and two-loop expressions \(\Pi^{(1)}\) and \(\Pi^{(2)}\), eqs. (1) and (7).
5 Comment on Threshold Effects far from the Threshold Region

In this section we want to comment on the use and the interpretation of the expression of the QED vacuum polarization function valid for all energies to $\mathcal{O}(\alpha^2)$ accuracy, eq. (17).

We have shown in Section 3 that the function $A$, which represents the resummed expression for diagrams with the instantaneous Coulomb exchange of two and more longitudinal polarized photons (in Coulomb gauge), see eq. (11), essentially has to be added to the one- and two-loop expressions for the vacuum polarization function in order to achieve $\mathcal{O}(\alpha^2)$ accuracy in the threshold region $|\beta| \lesssim \alpha$. Far from the threshold regime, however, $A$ represents contributions of order $\alpha^3$ and higher and therefore is irrelevant. This is what we mean by using the term “valid for all energies to $\mathcal{O}(\alpha^2)$ accuracy”. – But not more!

At this point the reader might be tempted to apply formula (17), as it stands, for an energy regime far from the threshold in the belief $A$ would represent higher-order information which should improve the accuracy of the one- and two-loop expressions calculated in the framework of conventional perturbation theory. Let us illustrate such a scenario for the energy regime where $q^2$ is close to zero. In this kinematic region, formula (17) can be expanded in terms of small $q^2$. Taking into account only the first non-vanishing contributions in $q^2/M^2$ and including only contribution up to $\mathcal{O}(\alpha^3)$ the result reads

$$\Pi^{\mathcal{O}(\alpha^2)}_{\text{QED}}(q^2) \underset{q^2 \rightarrow 0}{=} \left( \frac{\alpha}{\pi} \right) \frac{1}{15} \frac{q^2}{M^2} + \left( \frac{\alpha}{\pi} \right)^2 \frac{41}{162} \frac{q^2}{M^2} + \alpha^3 \frac{\pi^2}{48} \sqrt{\frac{q^2}{M^2}} + \mathcal{O}(\alpha^4), \tag{43}$$

where the numerical coefficient of the $\mathcal{O}(\alpha^3)$ coefficient is $\pi^2/48 = 0.21$. The corresponding multi-loop expression including also the first non-vanishing three-loop coefficient \[ prints reads

$$\Pi^{3\text{ loop}}_{\text{QED}}(q^2) \underset{q^2 \rightarrow 0}{=} \left( \frac{\alpha}{\pi} \right) \frac{1}{15} \frac{q^2}{M^2} + \left( \frac{\alpha}{\pi} \right)^2 \frac{41}{162} \frac{q^2}{M^2} + \alpha^3 \frac{\pi^2}{3} \left[ -\frac{8687}{13824} + \frac{\pi^2}{3} \left( \frac{1}{8} - \frac{1}{5} \ln 2 \right) + \frac{22781}{27648} \zeta_3 \right] \frac{q^2}{M^2} + \mathcal{O}(\alpha^4). \tag{44}$$

The numerical value of the constant term in the brackets is 0.32. It is evident that the $\mathcal{O}(\alpha^3)$ contributions which come from $\Pi^{\mathcal{O}(\alpha^2)}_{\text{QED}}$ and therefore contain information on the formation of positronium bound states are much larger than the three-loop contributions. The ratio between the former $\mathcal{O}(\alpha^3)$ contributions and the three-loop result even diverges for $q^2 \rightarrow 0$. The overall conclusion of this scenario would be that threshold (and therefore long-distance) effects dominate not only in the threshold regime but also the energy region $|q^2| \ll 4M^2$. This is obviously wrong! The “threshold effects” in eq. (13) contradict the Appelquist-Carrazone theorem and even represent contributions non-analytic at $q^2 = 0$. The solution to this apparent paradox is that $\Pi^{\mathcal{O}(\alpha^2)}_{\text{QED}}$ only describes the vacuum polarization function to $\mathcal{O}(\alpha^2)$ accuracy. All contributions of order $\alpha^3$ or higher have to ignored and do not represent proper higher-order contributions. This means that the contributions of the function $A$ are necessary to achieve $\mathcal{O}(\alpha^2)$ accuracy in the threshold region, but should be neglected if the vacuum polarization function has to evaluated far from the threshold point.

To make the latter point more explicit, let us imagine that the analytical form of the complete three-loop contributions to the vacuum polarization function would be known for all energies (in the same sense as the they are known for the one- and two-loop contributions, $\Pi^{(1)}$ and $\Pi^{(2)}$). We then...
could try to determine the expression for the vacuum polarization function valid to $\mathcal{O}(\alpha^3)$ accuracy for all energies in the same way as we have determined $\Pi_{\text{QED}}^{\mathcal{O}(\alpha^2)}$, which is valid to $\mathcal{O}(\alpha^2)$ accuracy for all energies. This would be achieved by matching the three-loop expression for the vacuum polarization function to the corresponding $\mathcal{O}(\alpha^3)$ formula calculated in NRQED in the same way as presented in Section 2. The vacuum polarization function valid to $\mathcal{O}(\alpha^3)$ accuracy for all energies would then have the form

$$
\Pi_{\text{QED}}^{\mathcal{O}(\alpha^3)}(q^2) = \left(\frac{\alpha}{\pi}\right) \Pi^{(1)}(q^2) + \left(\frac{\alpha}{\pi}\right)^2 \Pi^{(2)}(q^2) + \left(\frac{\alpha}{\pi}\right)^3 \Pi^{(3)}(q^2) + A(\alpha, \beta) - \alpha^3 \left[ i \frac{\pi^2}{24 \beta} \right] + \Delta(\alpha, \beta).
$$

In the second line of eq. (45) the contribution $\alpha^3 \left[ i \frac{\pi^2}{24 \beta} \right]$ has to be subtracted in order to avoid double counting in the threshold regime since

$$
\left(\frac{\alpha}{\pi}\right)^3 \Pi^{(3)}(q^2) \big|_{\beta \ll 1} \equiv \alpha^3 \left[ i \frac{\pi^2}{24 \beta} \right] + \mathcal{O}(\beta^0).
$$

It is therefore clear that far from threshold the second line of eq. (45) only contains contributions of order $\alpha^4$ and higher (see eq. (19)). Expanding now $\Pi_{\text{QED}}^{\mathcal{O}(\alpha^3)}$ for small values of $q^2$ would give a result identical to the three-loop expression, eq. (14). The large non-analytical $\mathcal{O}(\alpha^3)$ contribution which appeared in eq. (43) would be gone. It is obvious that this large contribution originates from the leading non-vanishing term of $\Pi^{(3)}$ in an expansion for $|\beta| \ll 1$ evaluated for small $q^2$. These contributions survive in $\Pi_{\text{QED}}^{\mathcal{O}(\alpha^2)}$, eq. (17), but are cancelled in $\Pi_{\text{QED}}^{\mathcal{O}(\alpha^3)}$, eq. (45). Using the same line of arguments it can easily be shown that all contributions of the function $A$ would be cancelled if formulae for the vacuum polarization function with successively higher accuracy would be determined.

The physical picture behind this cancellation can be drawn as follows: the contributions in function $A$ are generated by vacuum polarization diagrams with the instantaneous Coulomb exchange of two and more longitudinal photons, where the latter are defined in the Coulomb gauge. In the threshold region the exchange of these longitudinal photons represents the dominant effect, whereas all the other interactions, for simplicity reasons called “transverse” in the following, can be neglected in a first approximation. Although this approach is obviously not gauge invariant from the point of view of full quantum electrodynamics, the violation of gauge invariance is vanishing in the non-relativistic limit. This is not true, however, far from the threshold point. There, contributions from longitudinal and transverse photons are equally important. Their individual sizes are extraordinarily large but with different signs. Therefore, adding the transverse contributions to the contributions of function $A$ the greater part of the large corrections will be cancelled off, leaving results which can be obtained from conventional (multi-loop) perturbation theory. This remains true at any level of accuracy. From this picture it should be clear that neither effects from the formation of $e^+e^-$ bound states nor from the Coulomb rescattering, if the relative velocity of the $e^+e^-$ pair is much smaller than the speed of light, can ever lead to large corrections of the vacuum polarization function far from the threshold.

\footnote{In eq. (45) $\Delta(\alpha, \beta)$ denotes the $\mathcal{O}(\alpha^3)$ NRQED contributions, including the necessary subtractions in order to avoid double-counting. The actual form of these contributions is irrelevant here because we only want to discuss the large $\mathcal{O}(\alpha^3)$ contributions in eq. (43). However, it is straightforward to see that $\Delta$ contains terms of order $\alpha^3$ in the threshold regime, but is of order $\alpha^4$ far from the threshold point.}
region. There, the contributions of the function $A$ represent unphysical (and gauge non-invariant) contributions which cannot even be used to estimate the size of the real higher-order corrections.

We would like to remind the reader that the previous arguments are not applicable if a high number of derivatives of the vacuum polarization function below the threshold region is considered, $(d/dq^2)^n\Pi(q^2)$, $n \gg 1$. In the latter case threshold effects are essential. This can be easily understood from the relation

$$M_n(q^2) = \left( M^2 \frac{d}{dq^2} \right)^n \Pi(q^2) \sim M^{2n} \int \frac{dq^2}{q^2} \frac{\text{Im}\Pi(q^2)}{(q^2 - q^2)^n}. \quad (47)$$

For large $n$ and $|q^2| < 4M^2$ the high-energy contributions in the dispersion integration are strongly suppressed, which leads to the domination of effects coming from the threshold region. This fact is the foundation of QCD sum rule calculations. At this point we would like to take the opportunity to comment on a recent publication where QCD sum rules have been applied to extract $\alpha_s$ and the bottom quark mass from experimental data on the $\Upsilon$ resonances. In this publication it is claimed that $O(\alpha_s^2)$ corrections to the moments $M_n^{\text{QCD}}(0)$ have been calculated because two-loop corrections to the $b\bar{b}$ production cross section have been included into the analysis. It should be clear from the discussions of Section 4 that a two-loop calculation of the cross section is not sufficient to describe the $O(\alpha_s^2)$ corrections to the cross section in the threshold region. In the analysis of this can be easily seen from the fact that the removal of the two-loop contributions (after subtraction of the corresponding leading and next-to-leading threshold contributions) essentially has no effect on the results. The latter observation is taken as a “final test on the importance of higher-order corrections”. However, as shown in Section 4, the $O(\alpha_s^2)$ corrections to the cross section in the threshold region are expected to be at the 10% to 20% level and will therefore have a large impact on QCD sum rule calculations in the large $n$ limit. The mistake in the arguments is that it is implicitly assumed that the Sommerfeld factor, eq. (47), accounts for the resummation of all long-distance effects. Therefore all corrections to expression (48) should be calculable by fixed-order loop calculations alone. This is true for the $O(\alpha_s)$ short-distance correction factor $\left(1 - 4C_F\alpha_s/\pi\right)$, but this is not the case for higher-order corrections like $O(C_F^2\alpha_s^2)$ Darwin corrections calculated in Section 4. This fact will be demonstrated explicitly in a future publication, where all $O(C_F^2\alpha_s^2)$ corrections to the cross section will be presented. In this is it also assumed that the effects of the running of the strong coupling in the Sommerfeld factor can be determined by insertion of the effective running coupling $\alpha_V$, which is related to the short-distance corrections of the QCD potential [37, 38]. We would like to emphasize that this approach is not justified for large $n$ QCD sum rule calculations because the important saturation effects are neglected in this procedure. As a consequence the calculations presented in are not only not at the $O(\alpha_s^2)$ accuracy level but also include a systematic error at order $\alpha_s$ and therefore contain much larger uncertainties than presented there. The authors of finally criticize an older QCD sum rule calculation by Voloshin on the same subject, claiming that in the magnitude of higher-order corrections was underestimated. In this point we agree with the authors of because in it is assumed that $O(\alpha_s^2)$ corrections have “no enhancement” in the large $n$ limit and therefore should be of order $1/n$. This assumption is essentially equivalent to the statement that all $O(\alpha_s^2)$ corrections to the ground state Coulomb wave function at the origin of a bound $b\bar{b}$ pair should vanish. We have shown explicitly in this work that this assumption is not true by calculating the $O(C_F^2\alpha_s^2)$ Darwin corrections. The latter corrections amount to 10% to 20% for the

\footnote{If applied to QCD our conclusion is essentially equivalent to arguments employed in [35, 34].}
modulus squared of the ground state wave function at the origin for a bound $b\bar{b}$ pair and are far from being negligible. We therefore conclude that the results presented in [7] actually contain theoretical uncertainties at the 10% to 20% level, an order of magnitude larger than claimed there.

6 Summary

In this work we have used the concept of effective field theories to calculate the $O(\alpha^2)$ corrections to the QED vacuum polarization function in the threshold region and to define a renormalized version of the zero-distance Coulomb Green function. In the framework where non-relativistic quantum mechanics is part of an effective low energy field theory (NRQED), long-distance effects (coming from typical momentum scales below the electron mass) are determined completely by classical quantum mechanics calculations, whereas short-distance contributions (coming from momentum scales beyond the electron mass) are included via the matching procedure. For the latter contributions multi-loop techniques (in conventional covariant perturbation theory) have to be employed. We have demonstrated that the effective field theory approach represents a highly efficient method to merge sophisticated multi-loop methods with well-known textbook quantum mechanics time-independent perturbation theory. From the physical point of view this is achieved because the effective field theory concept allows for a transparent and systematic separation of long- and short-distance physics at any level of precision. For our calculations we have used a “direct matching” procedure which can be applied if the multi-loop results to the quantity of interest are at hand. This direct matching allows for a quite sloppy treatment of UV divergences in the effective field theory, but is of no value if calculations of quantities are intended for which no multi-loop expressions are available.

We have demonstrated the efficiency of our approach by calculating the $O(\alpha^6)$ “vacuum polarization” contributions to the positronium ground state hyperfine splitting without referring back to the Bethe-Salpeter equation, and by determining the $O(C_F^2\alpha_s^2)$ (next-to-next-to-leading order) Darwin corrections to heavy quark-antiquark bound state wave functions at the origin and to the heavy quark-antiquark production cross section in $e^+e^-$ annihilation (into a virtual photon). If the $O(C_F^2\alpha_s^2)$ Darwin corrections are taken as an order-of-magnitude estimate for the complete (yet unknown) $O(\alpha_s^2)$ corrections, the typical $O(\alpha_s^2)$ corrections for the $t\bar{t}$ production cross section can be expected at the few percent level for most of the threshold region. Around the 1S peak they might even amount to 5%. For the modulus squared of the ground state wave function of a bound $b\bar{b}$ pair (applicable to $\Upsilon(1S)$), the $O(C_F^2\alpha_s^2)$ Darwin corrections are between 10% and 20%, whereas the corresponding corrections for the $c\bar{c}$ system are between 15% and 35%. The uncertainties arise from the ignorance of higher-order corrections, in particular from the ignorance of the exact scale in the strong coupling. We conclude that the determination of all $O(\alpha_s^2)$ corrections would represent a considerable improvement of the present precision of theoretical calculations to the $t\bar{t}$ and $b\bar{b}$ system in the threshold region. For the $c\bar{c}$ system, on the other hand, this seems to be doubtful, a consequence of the large size of the strong coupling.

Finally, we have also discussed whether the formation of positronium states can lead to large corrections of the QED vacuum polarization function far from the threshold region and came to the conclusion that such corrections do not exist.
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