Vacuum polarization function to $O(\alpha^2)$ accuracy near threshold and Darwin corrections

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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 α^2 in size rather than α^2/π^2. The vacuum polarization effects in the single photon annihilation contributions to the $O(\alpha^6)$ hyperfine splitting of the positronium ground state are recalculated and an error in an older calculation is pointed out. The results are used to determine $O(C_F^2\alpha_s^2)$ (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 $t\bar{t}$ 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 Υ system is made. [S0556-2821(98)01303-4]

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I. INTRODUCTION

In recent years many sophisticated methods have been developed to calculate higher order (''multiloop'') 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 CERN e^+e^- collider 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 [1–4]. However, future experiments [Next Linear Collider (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

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

where M_Q is the heavy quark pole mass and $\sqrt{q^2}$ denotes the c.m. energy. In the process of heavy-quark–antiquark production above the threshold, $q^2>4M_Q^2$, β is equal to the velocity of the quarks in the c.m. frame. We therefore call β the ''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 nonperturbative effects (in the sense of ''not calculable analytically 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 α^n/β^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 nonrelativistic 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 complete knowledge of higher-order corrections would be extremely valuable. Most of the present analyses (see e.g. [5] for a review) 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 nonperturbative 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 Υ system [7],[1] 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 calcu-

[1]During completion of this paper we became aware of a new publication, where QCD sum rules for the Υ 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 Sec. V.

lated in a systematic way to in principle arbitrary order is nonrelativistic quantum chromodynamics (NRQCD), as formulated in [9], 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 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 multiloop calculations in the framework of conventional perturbation theory at the level of the intended accuracy. In this work we assume that the reader has some familiarity with the approach presented in [9].

In this work we demonstrate the efficient use of theoretical methods from NRQED [9] to calculate the QED vacuum polarization function in the threshold region to $O(\alpha^2)$ accuracy. We would like to emphasize that our result for the QED vacuum polarization function to $O(\alpha^2)$ accuracy in the threshold region, although completely derived from a number of older results, has never been presented in the literature before and therefore should be considered as new. In contrast to the standard matching procedure in NRQED [9], where the renormalization coefficients to the operators of the NRQED Lagrangian have to be determined explicitly, we match the unrenormalized NRQED expression for the vacuum polarization function to the corresponding QED results directly at the level of their analytical expressions. This ''direct matching'' approach considerably simplifies the calculations and leads to the same result as the standard matching procedure. We use our result to recalculate the vacuum polarization effects in the single photon annihilation contributions to the $O(\alpha^6)$ hyperfine splitting of the positronium ground state energy level without referring back to the Bethe-Salpeter equation. An error in an older calculation [10,11] on the same subject is pointed out. We analyze the vacuum polarization function at the bound state energies and above threshold and, in particular, concentrate on the size of the $O(\alpha^2)$ contributions. It is shown that the size of the $O(\alpha^2)$ contributions in the threshold regime is of order α^2 rather than α^2/π^2 which is a consequence of their long-distance character. In a second step our results for the QED vacuum polarization function in the threshold regime are applied to calculate $O(C_F^2\alpha_s^2)$ (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, $V_{\rm QCD}(r)=-C_F\alpha_s/r$, where the scale in the strong coupling is fixed. It is demonstrated that the size of the $O(C_F^2\alpha_s^2)$ Darwin corrections is also of order α_s^2 rather than α_s^2/π^2. We present simple physical arguments that the scale of the strong coupling governing the $O(C_F^2\alpha_s^2)$ Darwin corrections is of order $C_F\overline{M}_Q\alpha_s$ 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) $O(\alpha_s^2)$ corrections. The sign of the latter corrections and their actual numerical values can, of course, only be determined by an explicit calculation of all $O(\alpha_s^2)$ corrections. Finally, we address the question of whether bound state effects can lead to large corrections to the vacuum polarization function in kinematic regions far from the actual threshold regime. We come to the conclusion that such corrections do not exist.

At this point we want to emphasize that the approach presented in this work is not based on the Bodwin-Braaten-Lepage (BBL) factorization formalism [5] where bound state and threshold quantities involving heavy-quark–antiquark pairs are expressed as a sum of terms each of which consists of a product of a short-distance coefficient and a matrix element which incorporates long-distance and nonperturbative effects. In the BBL factorization formalism the short-distance coefficients can be determined using the standard matching procedure within NRQCD whereas the matrix elements have to be extracted from experimental data or lattice calculations. The spirit of this work is completely different. We entirely rely on the perturbative methods developed for NRQED [9,12] and transfer these techniques to heavy-quark–antiquark systems in QCD. The $O(C_F^2\alpha_s^2)$ Darwin corrections presented in this work therefore contain perturbative short- as well as long-distance contributions and represent first principles (i.e. not dependent on any model-like assumptions) QCD calculations. Of course, because we rely entirely on perturbative methods we cannot determine any nonperturbative effects. The only assumptions our approach is based on are that (i) the instantaneous (i.e. uncrossed) Coulomb-like exchange of longitudinal gluons (in Coulomb gauge) between the heavy quarks represents the dominant effect in the threshold regime and is the main reason for heavy-quark–antiquark bound state formation and that (ii) all further interactions and effects can be treated as a perturbation. We believe that the actual size of the $O(\alpha_s^2)$ corrections can then serve as an important *a posteriori* justification or falsification of these assumptions for the different heavy-quark–antiquark systems. Because we know that nonperturbative effects are much more important in the $c\bar{c}$ systems than in the $b\bar{b}$ and $t\bar{t}$ systems, a consequence of the ''smallness'' of the charm quark mass, we can expect that our perturbative approach contains much less predictive power for $c\bar{c}$ than for $b\bar{b}$ and $t\bar{t}$. This is confirmed by the size of the $O(C_F^2\alpha_s^2)$ Darwin corrections for the different heavy-quark–antiquark systems.

The program for this work is organized as follows: In Sec. II the calculation of the QED vacuum polarization function to $O(\alpha^2)$ accuracy in the threshold region is presented. We define a renormalized version of the Coulomb Green function for zero distances, which allows for the 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 $O(\alpha^2)$ accuracy. In Sec. III the

QED vacuum polarization function in the threshold region is analyzed with special emphasis on the size of the $O(\alpha^2)$ corrections, and the $O(\alpha^6)$ vacuum polarization effects in the single photon annihilation contributions to the positronium ground state hyperfine splitting are calculated. Section IV is devoted to the determination and analysis of the $O(C_F^2\alpha_s^2)$ 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 Sec. V we comment on the existence of threshold effects far from threshold and on recent QCD sum rule calculations for the Υ system [7,8]. Section VI contains a summary.

II. DETERMINATION OF THE QED VACUUM POLARIZATION FUNCTION IN THE THRESHOLD REGION TO $O(\alpha^2)$ ACCURACY

In this section we want to determine the QED vacuum polarization function to $O(\alpha^2)$ accuracy in the threshold regime where $|\beta| \lesssim \alpha$. In the following we present the necessary steps of consideration in order to arrive at this result. As already mentioned in Sec. I, all analytical ingredients needed to achieve this aim, the Green function of the nonrelativistic positronium Schrödinger equation and the one- and two-loop QED vacuum polarization functions (derived in the framework of conventional multiloop perturbation theory), can be found the in older literature. Therefore no details concerning the calculation of the latter three quantities are given here. The reader interested in the calculations of these results is referred to the references.

We consider the QED vacuum polarization function Π defined through the one-particle-irreducible current-current correlator

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

where $j^\mu(x) = ie\overline{\Psi}(x)\gamma^\mu\Psi(x)$ denotes the electromagnetic current. Ψ represents the Dirac field of the electron with charge e. According to the standard subtraction procedure, Π vanishes for $q^2 = 0$. It has been shown in a number of publications (see e.g. [13,14]) that in the nonrelativistic limit, i.e. taking into account only the dominant effects in the threshold region, the vacuum polarization function Π is directly related to the Green function $G_E^0(\vec{x},\vec{y})$ of the nonrelativistic positronium Schrödinger equation

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

where M is the electron (pole) mass, E denotes the energy relative to the threshold point, $E \equiv \sqrt{q^2} - 2M$, and α is the fine structure constant. Explicit analytic expressions for the Green function have been calculated in a number of classical papers [15]. The analytic expression for $G_E^0(\vec{x},0)$ is particularly simple and reads

$$\begin{aligned} G_E^0(\vec{x},0) &= \int \frac{d^3\vec{p}_0}{(2\pi)^3} e^{i\vec{p}_0\vec{x}} \frac{M_Q}{\vec{p}_0^2 - M^2\beta^2 - i\epsilon} \sum_{m=0}^{\infty} \prod_{n=1}^{m} \\ &\quad \times \int \frac{d^3\vec{p}_n}{(2\pi)^3} \frac{4\pi\alpha}{(\vec{p}_{n-1} - \vec{p}_n)^2} \frac{M_Q}{\vec{p}_n^2 - M^2\beta^2 - i\epsilon} \\ &= -i\frac{M^2\beta}{2\pi} e^{iM\beta r} \int_0^\infty e^{2iM\beta r t} \left(\frac{1+t}{t} \right)^{i\alpha/2\beta} dt, \end{aligned} \tag{4}$$

where $r \equiv |\vec{x}|$. The reader should note that in Eq. (4) we can identify $\beta = \sqrt{1 - 4M^2/(q^2 + i\epsilon)}$ with $\sqrt{(E + i\epsilon)/M}$ because we are only interested in $O(\alpha^2)$ accuracy in the threshold region. [For the same reason we replace the factor $1/q^2$ in the first line of Eq. (5) below by $1/(4M^2)$ in the second line of Eq. (5).] It can be easily seen from the first line of Eq. (4) that $G_E^0(0,0)$ represents the resummation of NRQED vacuum polarization diagrams with nonrelativistic electron-positron propagation and ladder-type instantaneous exchange of longitudinal polarized photons (called *Coulomb photons* in the following) in the Coulomb gauge to all orders in the coupling α [14]. The latter two effects constitute the dominant contributions contained in the NRQED Lagrangian [9] and are accounted for in the Schrödinger equation, Eq. (3).[2] For later reference we call the NRQED vacuum polarization diagrams resummed in $G_E^0(0,0)$ *nonrelativistic vacuum polarization diagrams*. In the threshold regime the proper relation between the vacuum polarization function Π, as defined in Eq. (2), and the Green function reads [13,14]

$$\begin{aligned} \Pi_{thr}^{0,O(\alpha^2)}(q^2) &= \frac{8\alpha\pi}{q^2} \lim_{r\to 0} G_E^0(\vec{x},0) \\ &= \alpha\left[\frac{1}{2Mr} + \frac{i}{2}\beta \right] + \alpha^2 \left[\frac{1}{2} - \gamma \right. \\ &\quad \left. - \frac{1}{2}\ln(-2iMr\beta) - \frac{1}{2}\Psi\left(1 - i\frac{\alpha}{2\beta} \right) \right], \end{aligned} \tag{5}$$

where γ is the Euler constant and Ψ represents the digamma function,

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

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

It is obvious that expression (5) contains contributions of $O(\alpha)$ and $O(\alpha^2)$. It can be easily checked that the two terms proportional to α and $\alpha\beta$ originate from the nonrelativistic vacuum polarization diagram without any photon exchange whereas the terms proportional to α^2 come from the sum of

[2] From this point of view the use of the Schrödinger equation (3) can be just regarded as a convenient tool to carry out the resummation of the NRQED diagrams.

all nonrelativistic vacuum polarization diagrams with one and more photon exchanges. The reader might ask why the nonrelativistic vacuum polarization diagrams with two and more photon exchanges do not result in contributions of order α^3 and higher. This can be easily understood from the fact that those nonrelativistic vacuum polarization diagrams lead to terms proportional to $\alpha^2(\alpha/\beta)^n$, n being the number of photons. The latter terms can be identified by expanding Eq. (5) for small α. Because we consider the kinematic regime $|\beta| \lesssim \alpha$, all those terms effectively contribute at the $O(\alpha^2)$ accuracy level; i.e. we count powers of β as powers of α. We will come back to this point later. Expression (5) further contains short-distance (UV) divergences for vanishing r in the $O(\alpha)$ and $O(\alpha^2)$ contributions. The divergence in the $O(\alpha)$ term comes from the nonrelativistic vacuum polarization diagram without any photon and the divergence in the $O(\alpha^2)$ term originates from the nonrelativistic vacuum polarization diagram with the exchange of one photon. The diagrams with two and more exchanges of photons are finite. The existence of these divergences comes from the fact that NRQED (and also nonrelativistic quantum mechanics) as an effective low energy theory 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. (5) by short distance (UV) divergences and has to be cured by matching NRQED to QED. In this light we have to regard expression (5) as unrenormalized, which we have indicated by using the superscripts 0.

Before carrying out the matching and renormalization procedure it is very instructive to examine whether there could be any relativistic effects in NRQED (i.e. from the low momentum regime) which might also contribute to the unnormalized vacuum polarization function $\Pi_{thr}^{0,O(\alpha^2)}$ at the $O(\alpha)$ or $O(\alpha^2)$ accuracy level. There are several possible sources of relativistic effects: relativistic corrections from the energy-momentum relation (i.e. corrections to the nonrelativistic kinetic energy in the NRQED Lagrangian), the Breit-Fermi $1/M^2$ corrections to the Coulomb interaction (like the Darwin term, spin-orbit interaction or the exchange of transverse photons in the instantaneous approximation[3]), relativistic corrections to the electron-positron production and annihilation vertex and the self-energy corrections to the electron and positron lines. Using textbook quantum mechanics time-independent perturbation theory one can show that the kinetic energy and Breit-Fermi corrections contribute at the $O(\alpha^3)$ and $O(\alpha^4)$ accuracy level.[4] The relativistic corrections from the electron-positron annihilation and production vertex, on the other hand, are proportional to $\lim_{r\to 0} \vec{\nabla}^2/M^2\, G_E^0(\vec{x},0)$ and [via the equation of motion (3)] also lead to $O(\alpha^3)$ and $O(\alpha^4)$ contributions. The electron and positron self-energy corrections, finally, lead to contributions beyond the $O(\alpha^2)$ level because they involve additional powers of α but no additional powers of $1/\beta$ which can only be generated by an exchange of a Coulomb photon between the electron and positron. As a consequence[5] expression (5) represents the complete unrenormalized NRQED vacuum polarization function to $O(\alpha^2)$ accuracy in the threshold regime which we have indicated by using the superscript $O(\alpha^2)$. At this point it should be noted that in the renormalized version of the vacuum polarization function [see Eq. (12)] the four relativistic effects mentioned above lead to constant (i.e. β-independent) $O(\alpha)$ and $O(\alpha^2)$ short-distance (i.e. high momentum) contributions. These effects, however, cannot be calculated within NRQED itself and will be included properly by the matching procedure which follows.

Let us now come to the question of renormalizing $\Pi_{thr}^{0,O(\alpha^2)}$ and the matching procedure. In the common approach to NRQED [9] the matching procedure for the vacuum polarization function would be carried out as follows: One considers the vacuum polarization contribution to the single photon annihilation scattering process $e^+e^- \to \gamma \to e^+e^-$ in the kinematic regime $\alpha \ll \beta \ll 1$. This regime corresponds to the elastic scattering of free and on-shell electrons and positrons, where the electron and positron velocity in the c.m. frame is much smaller than the speed of light but still much larger than the coupling α. The reader should note that the foundation of the matching procedure is that for $\alpha \ll \beta \ll 1$ both NRQED and conventional multiloop perturbation theory in QED are applicable[6] and therefore must lead to the same result. To achieve relative $O(\alpha^2)$ accuracy for the vacuum polarization contribution to the scattering process we have to expand the unrenormalized NRQED vacuum polarization function $\Pi_{thr}^{0,O(\alpha^2)}$, Eq. (5), for small α, identify the terms proportional to α, $\alpha\beta$ and α^2 and determine their contribution to the scattering amplitude.[7] Then the corresponding scattering contributions of the same

[3]In the threshold regime the dominant contribution from the exchange of transverse photons comes from the instantaneous (i.e. energy independent) component of the transverse photon propagator in momentum space [16].

[4]We would like to remind the reader that in the threshold regime $|\beta| \lesssim \alpha$ contributions of $O(\alpha^3)$ and $O(\alpha^4)$ correspond to multiloop terms proportional to $\alpha^n\beta^m$ with $n+m=3$ and 4, respectively, because for $|\beta| \lesssim \alpha$ we count powers of β as powers of α.

[5]The crossed exchange of Coulomb photons also represents an effect beyond the $O(\alpha^2)$ accuracy level because the instantaneous character of the exchange of Coulomb photons requires the propagation of the small component (from the Dirac spinor) of either the electron or the positron in the NRQED diagram. The process of the crossed exchange of Coulomb photons is therefore suppressed compared to the ladder-type exchange.

[6]For $\alpha \ll \beta \ll 1$ conventional perturbation theory in QED is valid because α represents the smallest parameter, whereas NRQED is valid because β is much smaller than the speed of light.

[7]As already mentioned before, the terms $\propto \alpha^2(\alpha/\beta)^n (n \geqslant 1)$ which are contained in $\Pi_{thr}^{0,O(\alpha^2)}$ in the limit $\alpha \ll \beta \ll 1$ are finite and, therefore, do not need to be renormalized. The reader should further note that the $O(\alpha)$ contributions of the renormalization coefficient multiplying the lowest order effective $(e^+e^-)(e^+e^-)$ four fermion interaction combined with the $O(\alpha)$ contribution of the unrenormalized NRQED vacuum polarization function also lead to $O(\alpha^2)$ contributions in the scattering amplitude.

order (i.e. leading and next-to-leading terms from the QED one-loop vacuum polarization and leading terms from the two-loop QED vacuum polarization for small β) have to be calculated in QED multiloop perturbation theory. The difference between the QED and the NRQED expression is β independent (and infrared safe) and uniquely determines the renormalization coefficient multiplying the NRQED $(e^+e^-)(e^+e^-)$ effective four fermion interaction describing the lowest order single photon annihilation process. This renormalization constant contains $O(\alpha)$ and $O(\alpha^2)$ UV-divergent and finite contributions which represent the short-distance corrections mentioned above and which render the NRQED scattering amplitude equal to the QED one. The renormalized and finite expression for the vacuum polarization function to $O(\alpha^2)$ accuracy in the threshold region is then obtained by finally combining the scattering contributions from the full unrenormalized vacuum polarization function $\Pi_{thr}^{0,O(\alpha^2)}$ with the $O(\alpha)$ and $O(\alpha^2)$ contributions from the renormalization constant and dividing the result by the leading order scattering amplitude.

However, we want to emphasize that the general matching procedure outlined above is only needed if the renormalization of the NRQED Lagrangian, i.e. an explicit determination of the renormalization constants of the various NRQED operators, is intended. If we are only interested in the renormalized expression of the vacuum polarization function in the threshold region, this procedure represents an unnecessary complication because for that we can match the terms proportional to α, $\alpha\beta$ and α^2 (for $\alpha \ll \beta \ll 1$) in $\Pi_{thr}^{0,O(\alpha^2)}$ to the corresponding one- and two-loop QED results directly at the level of their analytical expressions. This ''direct matching'' method leads to the same result as the conventional matching procedure will be described explicitly in the following: As already described above, we first have to identify the terms proportional to α, $\alpha\beta$ and α^2 from $\Pi_{thr}^{0,O(\alpha^2)}$ in the limit $\alpha \ll \beta \ll 1$,

$$\Pi_{thr}^{0,O(\alpha^2)}(q^2) \overset{\alpha\ll\beta}{=} \alpha\left[\frac{1}{2Mr}+\frac{i}{2}\beta\right]+\alpha^2\left[\frac{1}{2}-\frac{1}{2}\gamma - \frac{1}{2}\ln(-2iMr\beta)\right]+O\left(\frac{\alpha^3}{\beta}\right). \tag{6}$$

Then the one- and two-loop contributions to the vacuum polarization function in multiloop QED have to be determined in the same limit. The one- and two-loop contributions to Π, defined as

$$\Pi(q^2)=\Pi^{1\,\mathrm{loop}}(q^2)+\Pi^{2\,\mathrm{loop}}(q^2)+O\left(\left(\frac{\alpha}{\pi}\right)^3\right), \tag{7}$$

have been known for quite a long time for all energy and mass assignments [17–19]. In the limit $\beta \ll 1$ the one- and two-loop expressions read[8]

$$\Pi^{1\,\mathrm{loop}}(q^2) \overset{|\beta|\to 0}{=} \alpha\left[\frac{8}{9\pi}+\frac{i}{2}\beta\right]+O(\alpha\beta^2), \tag{8}$$

$$\Pi^{2\,\mathrm{loop}}(q^2) \overset{|\beta|\to 0}{=} \alpha^2\left[\frac{1}{4\pi^2}\left(3-\frac{21}{2}\zeta_3\right)+\frac{11}{32}-\frac{3}{4}\ln 2 - \frac{1}{2}\ln(-i\beta)\right]+O(\alpha^2\beta), \tag{9}$$

where $\zeta_3 = 1.202056903\ldots$. Comparing the contributions proportional to α and α^2 in expression (6) with Eqs. (8) and (9) and demanding equality we arrive at the following replacements for the divergences and constants in the unrenormalized vacuum polarization function $\Pi_{thr}^{0,O(\alpha^2)}$:

$$\frac{1}{2Mr}\to\frac{8}{9\pi}, \tag{10}$$

$$\frac{1}{2}-\frac{1}{2}\gamma-\frac{1}{2}\ln(2Mr)\to\frac{1}{4\pi^2}\left(3-\frac{21}{2}\zeta_3\right)+\frac{11}{32}-\frac{3}{4}\ln 2. \tag{11}$$

It should be noted that the expressions on the right-hand sides (RHS's) of Eqs. (10) and (11) represent the missing short-distance (i.e. high momentum) $O(\alpha)$ and $O(\alpha^2)$ contributions mentioned above and that it is therefore a necessary condition for the consistency of our approach that the RHS's of Eqs. (10) and (11) are β independent. In particular, the RHS of Eq. (10) represents the short-distance effects coming from the relativistic propagation of the electron-positron pair and from the relativistic electron-positron production and annihilation vertex, whereas the RHS of Eq. (11) represents short-distance contributions from the relativistic propagation of the electron-positron pair including the self-energy corrections, from the relativistic electron-positron production and annihilation vertex and from relativistic effects in the photon exchange (like from the transverse component of the photon propagator). At this point we would like to mention that compared to the conventional matching procedure in NRQED the ''direct matching'' described here has the advantage that the regularization of the UV divergences in the NRQED calculation can be performed in a quite sloppy way [see Eqs. (4), (5) and (6) where the regularization has been carried out by evaluating the Green function at a finite distance from the origin)]. That this does still lead to the correct renormalized result can be easily seen from the fact that the exact form of the constant terms on the LHS of the replacements (10) and (11) is completely irrelevant for the final expression of the renormalized vacuum polarization function. However, because the ''direct matching'' does not lead to a systematic determination of the NRQED renormalization constants, it can only be applied if a multiloop result in full QED of the quantity of interest is available. We would like to emphasize that the ''direct matching'' only relies on the existence of NRQED as a consistent effective field theory and that ''direct matching'' can also be applied to quantities which have a more complicated structure of UV divergences than $\Pi_{thr}^{0,O(\alpha^2)}$. Applying the replacements (10) and (11) to the unrenormalized NRQED vacuum polarization function $\Pi_{thr}^{0,O(\alpha^2)}$ we finally arrive at

[8]The reader should note that the two-loop QED vacuum polarization, Eq. (9), diverges logarithmically for vanishing β. This shows that beyond $O(\alpha)$ accuracy level conventional multiloop perturbation theory is inadequate for $|\beta| \lesssim \alpha$ indicating the need for the resummation contained in $\Pi_{thr}^{0,O(\alpha^2)}$, Eq. (6).

the following result for the renormalized vacuum polarization function to $O(\alpha^2)$ accuracy in the threshold region $|\beta| \lesssim \alpha$:

$$\Pi_{thr}^{O(\alpha^2)}(q^2) = \alpha\left[\frac{8}{9\pi} + \frac{i}{2}\beta\right] + \alpha^2\left[\frac{1}{4\pi^2}\left(3 - \frac{21}{2}\zeta_3\right) + \frac{11}{32} - \frac{3}{4}\ln 2 - \frac{1}{2}\ln(-i\beta)\right] + A(\alpha,\beta), \tag{12}$$

$$A(\alpha,\beta) \equiv -\frac{\alpha^2}{2}\left[\gamma + \Psi\left(1 - i\frac{\alpha}{2\beta}\right)\right], \tag{13}$$

which represents the main result of this work. $\Pi_{thr}^{O(\alpha^2)}$ is an analytical function and contains all short- and long-distance effects up to the $O(\alpha^2)$ accuracy level. Although all necessary ingredients to derive $\Pi_{thr}^{O(\alpha^2)}$ have been calculated a long time ago, $\Pi_{thr}^{O(\alpha^2)}$ has never been presented in this complete form in the literature before. Using the optical theorem it can be easily checked that $\Pi_{thr}^{O(\alpha^2)}$ correctly reproduces the well-known expression for the heavy lepton pair production cross section in e^+e^- annihilation in the nonrelativistic limit; see Eq. (36).

It is an interesting fact that the result for $\Pi_{thr}^{O(\alpha^2)}$ can be obtained directly from the one- and two-loop results, Eqs. (8) and (9), by the replacement

$$\ln(-i\beta) \to H(\alpha,\beta) \equiv \gamma + \ln(-i\beta) + \Psi\left(1 - i\frac{\alpha}{2\beta}\right) = \ln(-i\beta) - \frac{2}{\alpha^2}A(\alpha,\beta). \tag{14}$$

The function A resums the nonrelativistic vacuum polarization diagrams with exchange of two and more photons between the electron-positron pair and therefore represents the sum of the leading contributions for $\beta \to 0$ of all vacuum polarization diagrams with three and more loops in conventional QED perturbation theory. As we will see in Sec. III, the function A contains terms of order α^3 and higher for $\alpha \ll |\beta|$, where conventional perturbation theory is valid. However, if $|\beta| \lesssim \alpha$, then A is of order α^2. For $0 < \beta \ll \alpha$ the function A develops a logarithmic singularity

$$A(\alpha,\beta) \overset{|\beta|\ll\alpha}{=} \frac{\alpha^2}{2}\left[\ln\left(i\frac{2\beta}{\alpha}\right) - \gamma\right] + O(\alpha\beta), \tag{15}$$

which cancels the $\ln\beta$ singularity from the two-loop expression (9). At this point it is illustrative to examine the limits $\alpha \ll \beta$ and $\beta \ll \alpha$ for the function H, defined in Eq. (14), for real and positive values of β:

$$H(\alpha,\beta) \overset{\alpha\ll\beta}{=} \ln(-i\beta) + O\left(\frac{\alpha}{\beta}\right), \tag{16}$$

$$H(\alpha,\beta) \overset{\beta\ll\alpha}{=} \ln\left(\frac{\alpha}{2}\right) + \gamma - i\pi + O\left(\frac{\beta}{\alpha}\right). \tag{17}$$

It is evident that the function H interpolates between a $\ln\beta$ behavior in the region where conventional perturbation theory is valid and a constant with a logarithm of α for $\beta/\alpha \to 0$. This leads to a finite value for $\Pi_{thr}^{O(\alpha^2)}$ at the threshold point. As we will see in the next section, $\Pi_{thr}^{O(\alpha^2)}$ 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 [13].

Based on result (12) and the relation (5) we are now able to define a renormalized expression for the zero-distance Green function $G_E^0(0,0)$:

$$G_E^R(0,0) \equiv \frac{M^2}{2\alpha\pi}\,\Pi_{thr}^{O(\alpha^2)}(q^2). \tag{18}$$

As we will show in Secs. III and IV, 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 $O(\alpha^2)$ accuracy for all energies,

$$\Pi_{\rm QED}^{O(\alpha^2)}(q^2) = \Pi^{1\,\rm loop}(q^2) + \Pi^{2\,\rm loop}(q^2) + A(\alpha,\beta). \tag{19}$$

For the convenience of the reader we give the expressions for $\Pi^{1\,\rm loop}$ and $\Pi^{2\,\rm loop}$ valid for all energies [17–19],

$$\Pi^{1\,\rm loop}(q^2) = \left(\frac{\alpha}{\pi}\right)\left\{\frac{8-3\beta^2}{9} + \frac{\beta(3-\beta^2)}{6}\ln(-p)\right\}, \tag{20}$$

$$\begin{aligned}\Pi^{2\,\rm loop}(q^2) = \left(\frac{\alpha}{\pi}\right)^2\Bigg\{&\frac{18-13\beta^2}{24} + \frac{\beta(5-3\beta^2)}{8}\ln(-p) - \frac{(1-\beta)(33-39\beta-17\beta^2+7\beta^3)}{96}\ln(-p)^2 \\ &+ \frac{\beta(-3+\beta^2)}{3}\left[2\ln(1-p)\ln(-p) + \ln(-p)\ln(1+p) + \mathrm{Li}_2(-p) + 2\mathrm{Li}_2(p)\right] \\ &+ \frac{(3-\beta^2)(1+\beta^2)}{12}\left[2\ln(1-p)\ln(-p)^2 + \ln(-p)^2\ln(1+p) + 4\ln(-p)\mathrm{Li}_2(-p)\right. \\ &\left.+ 8\ln(-p)\mathrm{Li}_2(p) - 6\,\mathrm{Li}_3(-p) - 12\,\mathrm{Li}_3(p) - 3\zeta_3\right]\Bigg\},\end{aligned} \tag{21}$$

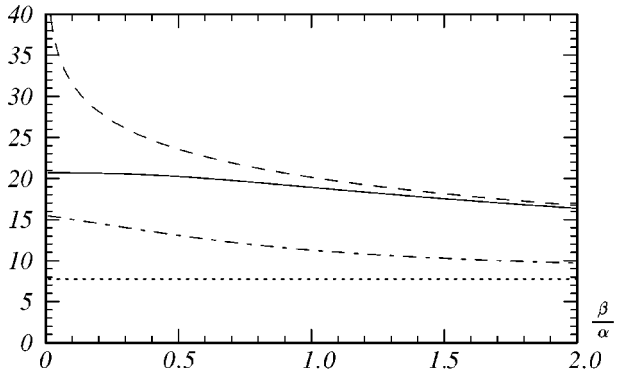

FIG. 1. The $O(\alpha^2)$ corrections to the vacuum polarization function in the threshold region with and without the contributions contained in the function A, Eq. (13), in the kinematic region $0<\beta<2\alpha$ above the threshold. The solid line denotes $\pi^2/\alpha^2\ \mathrm{Re}[\Pi^{2\,\mathrm{loop}}+A]$, the dashed line $\pi^2/\alpha^2\ \mathrm{Re}\,\Pi^{2\,\mathrm{loop}}$, the dashed-dotted line $\pi^2/\alpha^2\ \mathrm{Im}[\Pi^{2\,\mathrm{loop}}+A]$ and the dotted line $\pi^2/\alpha^2\ \mathrm{Im}\,\Pi^{2\,\mathrm{loop}}$. The value of the fine structure constant is taken as $\alpha=1/137$. $\Pi^{2\,\mathrm{loop}}$ represents the two-loop contribution to the vacuum polarization function and is displayed in Eqs. (9) and (21).

where

$$p\equiv\frac{1-\beta}{1+\beta}$$

and Li_2, Li_3 denote the di- and trilogarithms [20]. Expression (19) can be easily derived from $\Pi^{O(\alpha^2)}_{thr}$, Eq. (12), by replacing its one- and two-loop QED contributions in the limit $\beta\to 0$ [first line of Eq. (12)] by the corresponding one- and two-loop expression for all energies, Eqs. (20) and (21). Away from threshold, where conventional multiloop perturbation theory can be applied, $\Pi^{O(\alpha^2)}_{\mathrm{QED}}$ has $O(\alpha^2)$ accuracy because is contains the complete one- and two-loop QED vacuum polarization contributions and because the function A is of higher order; in the threshold region, on the other hand, $\Pi^{O(\alpha^2)}_{\mathrm{QED}}$ reduces to $\Pi^{O(\alpha^2)}_{thr}$ plus one- and two-loop contributions $\propto\alpha\beta^{n+1}$ and $\propto\alpha^2\beta^n$ $(n\geqslant 1)$, respectively, which represent terms beyond $O(\alpha^2)$ accuracy for $|\beta|\lesssim\alpha$. The reader should note that $\Pi^{O(\alpha^2)}_{\mathrm{QED}}$ vanishes at $q^2=0$ and is an analytic function in q^2 except at poles and branch cuts, and satisfies the dispersion relation

$$\Pi^{O(\alpha^2)}_{\mathrm{QED}}(q^2)=\frac{q^2}{\pi}\int_{-\infty}^{\infty}\frac{dq'^2}{q'^2}\frac{1}{q'^2-q^2-i\epsilon}\,\mathrm{Im}\,\Pi^{O(\alpha^2)}_{\mathrm{QED}}(q'^2). \tag{22}$$

The explicit form of $\mathrm{Im}\,\Pi^{O(\alpha^2)}_{\mathrm{QED}}$ in the threshold region will be presented in Sec. III. For the use and interpretation of formula (19) see also Sec. V.

III. EXAMINATION OF THE VACUUM POLARIZATION FUNCTION IN THE THRESHOLD REGION

In this section we analyze the properties of the vacuum polarization function for $|\beta|\ll 1$ above and below the threshold point $q^2=4M^2$. Compared to an older work on the same subject [13] 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 behavior of $\Pi^{O(\alpha^2)}_{thr}$. In particular, we focus on the size of the $O(\alpha^2)$ contributions. We also would like to mention that the vacuum polarization function has been studied in a similar way in [10]. In the latter publication, however, a different definition for the vacuum polarization is employed; only the positronium ground state energy is considered and the contribution proportional to $\alpha\beta$ is missing. We will come back to this point later. Comparing the methods used in [10] 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. (7)–(9), are reliable. This is consistent with the fact that the function A contains only contributions of order α^3 and higher,

$$\begin{aligned}A(\alpha,\beta)&\overset{\alpha\ll\beta}{=}\frac{\alpha^2}{2}\sum_{n=2}^{\infty}\zeta_n\left(i\frac{\alpha}{2\beta}\right)^{n-1}\\&=\alpha^3\left[\frac{i}{24}\frac{\pi^2}{\beta}\right]-\alpha^4\left[\frac{\zeta_3}{8\beta^2}\right]+O\left(\frac{\alpha^5}{\beta^3}\right).\end{aligned} \tag{23}$$

Thus, for practical applications in this kinematic region the contributions of the function A can be neglected. (See also the discussion in Sec. V.) One might think that for $\alpha\approx\beta$ the one- and two-loop expressions should still represent an appropriate $O(\alpha^2)$ prediction, because the radius of convergence of the series on the RHS of Eq. (23) is $|\beta|=\alpha/2$ [21]. However, as illustrated in Fig. 1, for $\alpha\approx\beta$ the contributions coming from the function A are already of order α^2/π^2 and thus should be included if $O(\alpha^2)$ 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 $\Pi^{2\,\mathrm{loop}}$; see Eqs. (9) and (15). Therefore the value of $\Pi^{O(\alpha^2)}_{thr}$ at the threshold point is finite and reads[9] $(\alpha=1/137)$

$$\begin{aligned}&\Pi^{O(\alpha^2)}_{thr}(q^2\to 4M^2+)\\&=\left(\frac{\alpha}{\pi}\right)\frac{8}{9}+\alpha^2\left[-\frac{1}{2}\ln\,\alpha-\frac{1}{2}\gamma\right.\\&\quad\left.+\frac{1}{4\,\pi^2}\left(3-\frac{21}{2}\zeta_3\right)+\frac{11}{32}-\frac{1}{4}\ln 2+i\frac{\pi}{2}\right]\\&=0.89\left(\frac{\alpha}{\pi}\right)+\left(-0.36-\frac{1}{2}\ln\,\alpha+i\frac{\pi}{2}\right)\alpha^2\\&=0.89\left(\frac{\alpha}{\pi}\right)+\left(2.10+i\frac{\pi}{2}\right)\alpha^2.\end{aligned} \tag{24}$$

[9]The plus sign in the argument of $\Pi^{O(\alpha^2)}_{thr}$, Eq. (24), indicates that the expression on the RHS of Eq. (24) represents only a right-sided limit on the real q^2 axis.

It is evident from Eq. (24) and Fig. 1 that the size of the $O(\alpha^2)$ corrections in the threshold region is of order α^2 rather than α^2/π^2, whereas the $O(\alpha)$ contribution is of order α/π. This can be understood from the fact that the $O(\alpha)$ contribution in $\Pi_{thr}^{O(\alpha^2)}$ comes entirely from the one-loop result $\Pi^{1\,\mathrm{loop}}$, Eq. (8), and therefore originates from momenta beyond the scale of the electron mass. High momenta contributions are expected to be of order α/π if no ''large logarithms'' occur.[10] The large $O(\alpha^2)$ contributions to $\Pi_{thr}^{O(\alpha^2)}$, on the other hand, arise from the interplay of the logarithm of the velocity in $\Pi^{2\,\mathrm{loop}}$, Eq. (9), 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 $\Pi^{2\,\mathrm{loop}}$. We therefore conclude that the large $O(\alpha^2)$ contributions are of long-distance origin. This is particularly obvious for the $\ln\alpha$ term which could never be generated at short distances.[11] At this point it is mandatory to mention that the phenomenon that the perturbative series for threshold and bound state quantities is often an expansion in α rather than α/π can be observed throughout the literature and the textbooks on this subject. A well-known example is the perturbative series describing the energy levels of the Hydrogen atom. Nevertheless, we find it important to emphasize this phenomenon here in order to illustrate the different behavior of perturbation theory for bound state and threshold quantities compared to high energy processes and to prepare for the large numerical size of the $O(\alpha_s^2)$ corrections calculated in Sec. IV.

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. (7)–(9), provide a viable prediction, because the contributions from the function A are of order α^3 and higher. They are beyond the intended accuracy and can be neglected. (See also the discussion in Sec. V.) 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,

$$\beta = i\frac{\alpha}{2n} \Leftrightarrow E = -\frac{M\alpha^2}{4n^2} \quad (n=1,2,3,\ldots), \tag{25}$$

because the vacuum polarization function is expected to have poles at those energy values. Therefore the full expression for $\Pi_{thr}^{O(\alpha^2)}$, Eq. (12), must be employed. It is straightforward to check that $\Pi_{thr}^{O(\alpha^2)}$ indeed has poles at the positronium energy levels [13], leading to the following Laurent expansion at the bound state energies $E_n = -M\alpha^2/4n^2$ $(n=1,2,3,\ldots)$,

$$\lim_{E\to E_n} \Pi_{thr}^{O(\alpha^2)}(q^2) = \frac{M\alpha^4}{4n^3}\frac{1}{E_n - E - i\epsilon} + \left(\frac{\alpha}{\pi}\right)\frac{8}{9} + \alpha^2[a_n] + O(E_n - E), \tag{26}$$

where

$$a_n \equiv -\frac{1}{2}\ln\alpha + \frac{1}{2}\left[\frac{1}{n} + \ln n - \sum_{i=1}^{n-1}\frac{1}{i}\right] + \frac{1}{4\pi^2}\left(3 - \frac{21}{2}\zeta_3\right) + \frac{11}{32} - \frac{1}{4}\ln 2. \tag{27}$$

For completeness we also present the corresponding Laurent expansion for the renormalized zero-distance Green function based on definition (18),

$$\lim_{E\to E_n} G_E^R(0,0) = \frac{|\Psi_n(0)|^2}{E_n - E - i\epsilon} + \frac{4}{9}\frac{M^2}{\pi^2} + \frac{M^2\alpha}{2\pi}[a_n] + O(E_n - E). \tag{28}$$

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

$$|\Psi_n(0)|^2 = \frac{M^3\alpha^3}{8\pi n^3}. \tag{29}$$

In Eqs. (26)–(28) 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 $O(\alpha^2)$ corrections in these constant terms is [similar to the $O(\alpha^2)$ contributions above threshold] of order α^2 rather than α^2/π^2, indicating again the long-distance character of the $O(\alpha^2)$ corrections. In Table I 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,

$$\lim_{n\to\infty}\alpha^2[a_n] = \alpha^2\left[-\frac{1}{2}\ln\alpha - \frac{1}{2}\gamma + \frac{1}{4\pi^2}\left(3 - \frac{21}{2}\zeta_3\right) + \frac{11}{32} - \frac{1}{4}\ln 2\right], \tag{30}$$

TABLE I. 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	∞
a_n	2.89	2.48	2.35	2.29	2.25	2.10

[10]For comparison the reader might consider the well-known one- and two-loop contributions to the anomalous magnetic moment of the electron [18,22], $g_e - 2 = (\alpha/\pi) - 0.66(\alpha/\pi)^2 + O((\alpha/\pi)^3)$. Here, long-distance effects from the e^+e^- threshold do not play any role. Therefore $g_e - 2$ can be regarded as a typical short-distance quantity with no ''large logarithms.''

[11]As explained during the matching procedure carried out in Sec. II, the $O(\alpha^2)$ contributions of $\Pi_{thr}^{O(\alpha^2)}$ actually contain short- and long-distance effects. Although a separation between both types of effects is in general scheme dependent, it is fair to say that the long-distance contributions are dominating in size compared to the short-distance ones for a reasonable separation scheme. It is therefore justified to regard the $O(\alpha^2)$ contributions as long-distance dominated as far as their numerical size is concerned.

and coincides with the $O(\alpha^2)$ contributions of $\mathrm{Re}\,\Pi_{thr}^{O(\alpha^2)}(q^2 \to 4M^2+)$, Eq. (24). The numerical value for $\lim_{n\to\infty} a_n$ is also presented in Table I.

To illustrate the importance of the constants a_n in time-independent perturbation theory (TIPT), we recalculate the $O(\alpha^6)$ vacuum polarization effects in the single photon annihilation contributions to the ground state triplet-singlet hyperfine splitting (HFS) of the positronium, which were, to our knowledge, considered for the first time in [10,11]. These 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 δ-function kernel in the configuration-space representation (corresponding to a constant kernel in momentum space) with the form

$$H_{ann}(\vec{x})=\frac{2\alpha\pi}{M^2}\,\delta^{(3)}(\vec{x}), \tag{31}$$

which represents a relativistic correction to the nonrelativistic Hamiltonian in Eq. (3). $H_{ann}(\vec{x})$ can now be used in TIPT. Taking into account that $\Pi_{thr}^{O(\alpha^2)}$ contains $O(\alpha)$ as well as $O(\alpha^2)$ contributions we have to apply second- and third-order TIPT to obtain all relevant $O(\alpha^6)$ contributions to the HFS. The formal result for the $O(\alpha^6)$ energy shift for the triplet states with radial quantum numbers n and with $l=0$ due to H_{ann} reads

$$\delta E_{ann,n}^{\alpha^6}=\left\{ \sum\!\!\!\!\!\!\int_{l\neq n} \langle n|H_{ann}\frac{|l\rangle\langle l|}{E_n-E_l}H_{ann}|n\rangle + \sum\!\!\!\!\!\!\int_{m\neq n}\ \sum\!\!\!\!\!\!\int_{k\neq n} \langle n|H_{ann}\frac{|m\rangle\langle m|}{E_n-E_m}H_{ann}\frac{|k\rangle\langle k|}{E_n-E_k} \times H_{ann}|n\rangle \right\}_{O(\alpha^6)}, \tag{32}$$

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 $\{\}_{O(\alpha^6)}$ indicates that only $O(\alpha^6)$ 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 $\delta E_{ann,n}^{\alpha^6}$,

$$\sum\!\!\!\!\!\!\int_{l\neq n}\langle 0|\frac{|l\rangle\langle l|}{E_l-E_n}|0\rangle=\sum\!\!\!\!\!\!\int_{l\neq n}\frac{|\Psi_l(0)|^2}{E_l-E_n} =\lim_{E\to E_n}\left[G_E^0(0,0)-\frac{|\Psi_n(0)|^2}{E_n-E-i\epsilon}\right]. \tag{33}$$

However, relation (33) still contains divergences [see Eq. (5)]. As we have pointed out in Sec. II, these divergences indicate that nonrelativistic quantum mechanics is not capable of describing 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 (33) by its renormalized version $G_E^R(0,0)$, Eq. (18) [using Eq. (12)], which describes short-distance physics properly. The final expression for $\delta E_{ann,n}^{\alpha^6}$ then reads

$$\begin{aligned}\delta E_{ann,n}^{\alpha^6}&=|\Psi_n(0)|^2\left\{\left[\frac{2\alpha\pi}{M^2}\right]^2\left(-\frac{M^2\alpha}{2\pi}a_n\right)+\left[\frac{2\alpha\pi}{M^2}\right]^3\left(-\frac{4}{9}\frac{M^2}{\pi^2}\right)^2\right\}\\ &=\frac{M\alpha^6}{4n^3}\left\{\frac{1}{2}\ln\alpha-\frac{1}{2}\left(\frac{1}{n}+\ln n-\sum_{i=1}^{n-1}\frac{1}{i}\right)+\frac{1}{4\pi^2}\left(\frac{13}{81}+\frac{21}{2}\zeta_3\right)-\frac{11}{32}+\frac{1}{4}\ln 2\right\}.\end{aligned} \tag{34}$$

For the ground state ($n=1$) the $O(\alpha^6)$ vacuum polarization contribution to the HFS then reads

$$\delta E_{ann,1}^{\alpha^6}=\frac{M\alpha^6}{4}\left\{\frac{1}{2}\ln\alpha+\frac{1}{4\pi^2}\left(\frac{13}{81}+\frac{21}{2}\zeta_3\right)-\frac{27}{32}+\frac{1}{4}\ln 2\right\}. \tag{35}$$

Our result differs from the one presented in [10,11][12] by the amount $M\alpha^6/16$. The discrepancy comes from the fact that in [10,11] the contribution proportional to $\alpha\beta$ in the one-loop vacuum polarization has not been taken into account.[13]

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 $\Pi_{thr}^{O(\alpha^2)}$ by means of the optical theorem [14,23],

$$\begin{aligned}R_{thr}^{L^+L^-}&=\frac{\sigma(e^-e^+\to\gamma^*\to L^+L^-)}{\sigma_{pt}}\\ &=\frac{3}{\alpha}\,\mathrm{Im}\,\Pi_{thr}^{O(\alpha^2)}(q^2)=\frac{6\pi}{M^2}\,\mathrm{Im}\,G_E^R(0,0)\\ &=\frac{6\pi^2}{M^2}\sum_{n=1}^{\infty}|\Psi_n(0)|^2\delta(E-E_n)+\Theta(E)\frac{3}{2}\frac{\alpha\pi}{1-\exp\left(-\frac{\alpha\pi}{\beta}\right)},\end{aligned} \tag{36}$$

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[12] In [11] the authors corrected an error in the result presented in [10]. In our comparison we refer to the corrected result from [11].

[13] This can be easily seen by comparing Eq. (33) of [10] with Eq. (8) in this work for

$$q_{n=1}^2=\left(2M-\frac{M\alpha^2}{4}\right)^2\Leftrightarrow\beta_{n=1}=i\frac{\alpha}{2}+O(\alpha^3).$$

This shows that at bound state energies the one-loop contribution to the vacuum polarization function also contains terms of order α^2.

where σ_{pt} represents the point cross section and only final-state interactions are taken into account.

IV. DARWIN CORRECTIONS IN QCD

In the previous section we have shown that the size of the $O(\alpha^2)$ corrections to the QED vacuum polarization function in the threshold region is of order α^2 rather than α^2/π^2. Although this fact is important for precision tests of QED,[14] it does not lead to theoretical concerns about the convergence of the perturbative series because of the smallness of the fine structure constant α 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 α_s^2 rather than α_s^2/π^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 do 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 nonrelativistic quark-antiquark system described by a Schrödinger equation with the QCD potential $V_{QCD}(r) = -C_F\,\alpha_s/r$, where $C_F=(N_c^2-1)/2N_c=4/3$.

The Darwin interaction is generated in the nonrelativistic expansion of the Dirac equation. In the configuration-space representation it is proportional to a δ function and reads[15]

$$H_{Dar}(\vec{x}) = \frac{C_F\alpha_s\pi}{M_Q^2}\,\delta^{(3)}(\vec{x}). \tag{37}$$

A practical application for the corrections to the bound state wave functions at the origin is the leptonic decay rate of the J/ψ and the $\Upsilon(1S)$ and (maybe) of the first few excited states of the Υ family, whereas the corrections to the cross section would be relevant for $t\bar{t}$ production at the NLC. We explicitly mention those applications in this context because it is believed that for them nonperturbative (in the sense ''not calculable analytically from first principles in QCD'') effects are either well under control or even negligible [25,14]. 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 nonperturbative 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 $\alpha\to C_F\alpha_s$. It is then straightforward to determine the $O(C_F^2\alpha_s^2)$ Darwin corrections to the modulus squared of the $l=0$ bound state wave functions at the origin ($n=1,2,3,\ldots$),

$$\delta|\Psi_n^{\rm QCD}(0)|^2_{Dar} = -2|\Psi_n^{\rm QCD}(0)|\left\{\frac{C_F\alpha_s\pi}{M_Q^2}\lim_{E\to E_n^{\rm QCD}}\left[G_E^{R,{\rm QCD}}(0,0)-\frac{|\Psi_n^{\rm QCD}(0)|^2}{E_n^{\rm QCD}-E-i\epsilon}\right]\right\}_{O(C_F^2\alpha_s^2)} = -|\Psi_n^{\rm QCD}(0)|^2C_F^2\alpha_s^2a_n^{\rm QCD}, \tag{38}$$

[14]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 O(α) (next-to-leading order) accuracy level. This can be easily seen from the fact that the complete threshold region for the $\tau^+\tau^-$ system, $|\beta| \lesssim \alpha \Leftrightarrow |\sqrt{q^2}-2m_\tau| \lesssim m_\tau\alpha^2=0.1$ MeV, still lies within the limits on the tau mass itself, $m_\tau=1777.00^{+0.30}_{-0.27}$ MeV [24]. Thus only experiments on electron and muon systems can be regarded as precision tests of QED in the threshold regime.

[15]Compared to the Darwin interaction known from the hydrogen atom the expression on the RHS of Eq. (37) is a factor of 2 larger because both quark-antiquark-gluon vertices involved in the gluon exchange contribute.

where the symbol $\{\}_{O(C_F^2\alpha_s^2)}$ indicates that only $O(C_F^2\alpha_s^2)$ corrections are taken into account.[16] The calculation of the $O(C_F^2\alpha_s^2)$ Darwin corrections to the quark-antiquark cross section in the threshold region is more involved. Here, we apply the optical theorem, Eq. (36), to the corrections of the zero-distance Green function themselves:

$$\delta G_{E,Dar}^{R,\mathrm{QCD}}(0,0) = -\frac{C_F\alpha_s\pi}{M_Q^2}[G_E^{R,\mathrm{QCD}}(0,0)]^2. \tag{39}$$

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

$$\begin{aligned}\delta R_{thr,Dar}^{Q\bar{Q}} &= N_c e_Q^2 \frac{6\pi}{M_Q^2}\,\mathrm{Im}\; G_E^{R,\mathrm{QCD}}(0,0) \\ &\quad\times\left\{-\frac{2C_F\alpha_s\pi}{M_Q^2}\,\mathrm{Re}\; G_E^{R,\mathrm{QCD}}(0,0)\right\}_{O(C_F^2\alpha_s^2, C_F\alpha_s\beta)} \\ &= R_{thr}^{Q\bar{Q}}\{-\mathrm{Re}\;\Pi_{thr}^{O(C_F^2\alpha_s^2),\mathrm{QCD}}(q^2)\}_{O(C_F^2\alpha_s^2, C_F\alpha_s\beta)},\end{aligned} \tag{40}$$

where $R_{thr}^{Q\bar{Q}}$ represents the ''Sommerfeld factor'' (sometimes also called the ''Fermi factor''),

$$\begin{aligned}R_{thr}^{Q\bar{Q}} &= N_c e_Q^2\,\frac{6\pi}{M_Q^2}\,\mathrm{Im}\; G_E^{R,\mathrm{QCD}}(0,0) \\ &= N_c e_Q^2 \frac{3}{2}\,\frac{C_F\alpha_s\pi}{1-\exp\left(-\dfrac{C_F\alpha_s\pi}{\beta}\right)} \\ &= N_c e_Q^2 \frac{3}{2}\beta\,\exp\left(\frac{C_F\alpha_s\pi}{2\beta}\right)\Gamma\left(1+i\frac{C_F\alpha_s}{2\beta}\right)\Gamma\left(1-i\frac{C_F\alpha_s}{2\beta}\right)\end{aligned} \tag{41}$$

and e_Q denotes the electric charge of the heavy quark. Below threshold we have to determine the corrections to the residues of $G_E^{R,\mathrm{QCD}}(0,0)$ 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. (38). It is an interesting fact that Eq. (40) 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. (41), and the contribution involving the digamma function of the $O(C_F^2\alpha_s^2)$ Darwin corrections above threshold [see Eqs. (13), (12) and (40)] as

$$\begin{aligned}&R_{thr}^{Q\bar{Q}}\left\{1+\frac{C_F^2\alpha_s^2}{4}\left[\Psi\left(1+i\frac{C_F\alpha_s}{2\beta}\right)+\Psi\left(1-i\frac{C_F\alpha_s}{2\beta}\right)\right]\right\} \\ &\quad\to N_c e_Q^2\frac{3}{2}\beta\,\exp\left(\frac{C_F\alpha_s\pi}{2\beta}\right)\Gamma\left(\frac{C_F^2\alpha_s^2}{4}+1+i\frac{C_F\alpha_s}{2\beta}\right) \\ &\quad\times\Gamma\left(\frac{C_F^2\alpha_s^2}{4}+1-i\frac{C_F\alpha_s}{2\beta}\right).\end{aligned} \tag{42}$$

It can be easily checked that the function $\Gamma(C_F^2\alpha_s^2/4+1-i\,C_F\alpha_s/2\beta)$ develops poles at the energies[17]

$$\tilde{E}_n^{\mathrm{QCD}} \equiv E_n^{\mathrm{QCD}} + \delta E_{n,Dar}^{\mathrm{QCD}} \quad (n=1,2,3,\ldots), \tag{43}$$

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

$$\begin{aligned}\delta E_{n,Dar}^{\mathrm{QCD}} &= \langle n^{\mathrm{QCD}}|H_{Dar}|n^{\mathrm{QCD}}\rangle \\ &= |\Psi_n^{\mathrm{QCD}}(0)|^2\frac{C_F\alpha_s\pi}{M_Q^2} = \frac{M_Q C_F^4\alpha_s^4}{8n^3}.\end{aligned} \tag{44}$$

At this point we also want to emphasize that the $\ln(C_F\alpha_s)$ and digamma contributions occurring in Eqs. (38) and (40) are not related to the running of the strong coupling. These 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 $\propto C_F\alpha_s M_Q$ [27]. So far no renormalization group argument has been found to determine these logarithmic terms to all orders in α in the sense of a leading logarithmic resummation. It should also be noted that there also exist $\ln(C_F\alpha_s)$ contributions induced by the running of the strong coupling. The determination of these contributions to the $O(\alpha_s^2)$ corrections to the wave functions and the cross section in the threshold region is beyond the scope of this work and will be addressed in a future publication. The $\ln(C_F\alpha_s)$ contributions to the $O(\alpha_s)$ corrections induced by the running of the strong coupling have been discussed in [28,25].

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 $O(\alpha_s^3)$ analysis, which is beyond the scope of this work. However, one can find simple arguments that the scale in the strong couplings of expressions (38) and (40) 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 $|\Psi_n^{\mathrm{QCD}}(0)|^2$ and $R_{thr}^{Q\bar{Q}}$ 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

[16] Equation (38) also generates $O(C_F\alpha_s)$ corrections which differ from the well-known $O(C_F\alpha_s)$ corrections generated by the $(1-4C_F\alpha_s/\pi)$ correction factor [26]. Adding up all the $O(C_F\alpha_s)$ 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. (40).

[17] 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.

TABLE II. The relative $\mathcal{O}(C_F^2\alpha_s^2)$ 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 $c\bar{c}$ systems, respectively. Displayed are the smallest and largest values for the range of α_s values given below Eq. (45) for the radial quantum numbers $n=1$, 2, 3, 4 and for $n\to\infty$.

n	1	2	3	4	∞
$\Delta^{t\bar{t}}_{\Psi,n}$	$-0.05/-0.04$	$-0.04/-0.03$	$-0.03/-0.02$	$-0.03/-0.02$	$-0.02/-0.02$
$\Delta^{b\bar{b}}_{\Psi,n}$	$-0.20/-0.11$	$-0.09/-0.06$	$-0.06/-0.05$	$-0.05/-0.04$	$-0.02/+0.01$
$\Delta^{c\bar{c}}_{\Psi,n}$	$-0.34/-0.17$	$-0.10/-0.09$	$-0.06/-0.01$	$-0.05/+0.03$	$-0.01/+0.15$

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 [28,25]; i.e. the scale of the strong coupling is of order $C_F\alpha_s M_Q$ although the kinematic relative momentum of the quark pair vanishes.[18] 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 α_s comes from the Darwin interaction H_{Dar}, and the other power of α_s (including the $\ln(C_F\alpha_s)$ terms) originates from the $O(\alpha_s^2)$ contribution of the vacuum polarization function $\Pi_{thr}^{O(C_F^2\alpha_s^2),\mathrm{QCD}}$. As mentioned in the previous section, the latter contribution is mainly 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 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. (38) and (40) can therefore be estimated via the self-consistency equation

$$\alpha_s=\alpha_s(C_F\alpha_s M_Q), \tag{45}$$

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 modified minimal subtraction scheme ($\overline{\mathrm{MS}}$) definition for the strong coupling, the one-loop QCD beta function and $\alpha_s(M_z=91.187\ \mathrm{GeV})=0.125$ and by taking twice and half the argument of the strong coupling on the RHS of relation (45). Further, the mass values in Eq. (45) have been taken to be the pole values. For the quark (pole) masses we have chosen $M_t=175$ GeV, $M_b=5$ GeV and $M_c=1.7$ 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 α_s might result. This dependence on the prescription is particularly strong for the charm system.[19] 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 $t\bar{t}$ 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.

In Table II 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 $\Delta_{\Psi,n}\equiv\delta|\Psi_n^{\mathrm{QCD}}(0)|^2_{Dar}/|\Psi_n^{\mathrm{QCD}}(0)|^2$ 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. (45). 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 α_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 $O(C_F^2\alpha_s^2)$ Darwin corrections to the (stable) quark-antiquark production cross section

[18] In [28,25] a proof for saturation is only given for the cross section above the threshold point. An analogous proof for a highly excited state or the cross section slightly below the threshold point does, to our knowledge, not exist in the literature. Such a proof is, however, much more 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. [25]). 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.

[19] 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 and charm systems, 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.

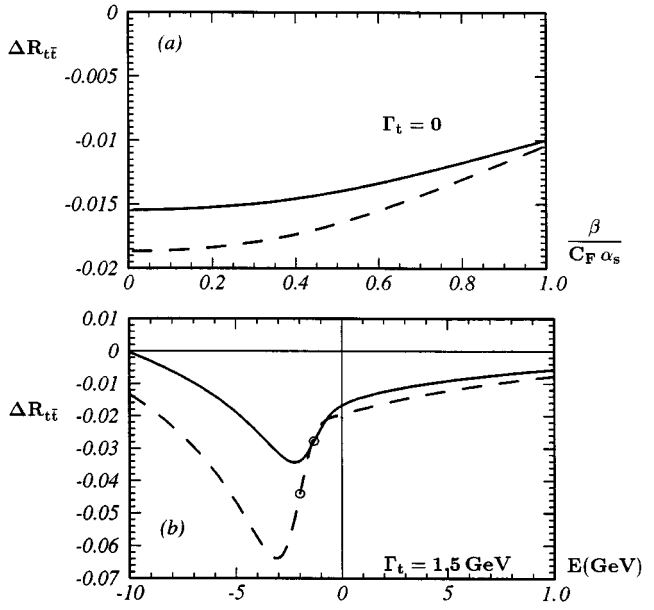

FIG. 2. The relative $O(C_F^2\alpha_s^2)$ Darwin corrections to the $t\bar{t}$ production cross section in the threshold region for the cases $\alpha_s = 0.13$ (solid lines) and 0.16 (dashed lines) for stable (a) and unstable (b) top quarks. The circles in (b) indicate the location of the $1S$ Coulomb energy level.

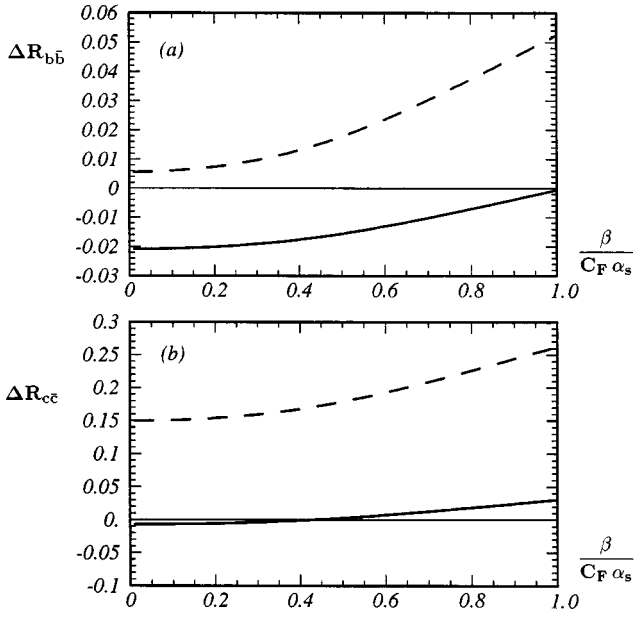

FIG. 3. The relative $O(C_F^2\alpha_s^2)$ Darwin corrections to the $b\bar{b}$ (a) and $c\bar{c}$ (b) production cross section in the kinematic region $0<\beta<C_F\alpha_s$ above threshold. The solid line corresponds to $\alpha_s=0.25$ (0.34) and the dashed line to $\alpha_s=0.38$ (0.59) for the case of $b\bar{b}$ ($c\bar{c}$) production.

$\Delta R_{Q\bar{Q}} \equiv \delta R^{Q\bar{Q}}_{thr,Dar}/R^{Q\bar{Q}}_{thr}$ 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) α_s value given below Eq. (45). 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 α_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 occur for larger velocities. In contrast to the top system the dependence of the corrections on the changes in the α_s value (3% for $\beta=0$ 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 α_s is 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 $\Gamma_t=1.5$ GeV (see Fig. 2b) in the energy range -10 GeV$<E<+10$ GeV in order to demonstrate the impact of the large top quark width on the $O(C_F^2\alpha_s^2)$ Darwin corrections. This has been achieved by the naive replacement $E\rightarrow E+i\Gamma_t$ in Eqs. (40) and (41). We want to mention that the inclusion of a finite width by this naive procedure does not represent a consistent treatment at the $O(\alpha_s^2)$ accuracy level. However, we find that this approach is justified here in order to demonstrate that the typical size of the $O(C_F^2\alpha_s^2)$ Darwin corrections is not altered if the top quark width is taken into account. In this case the relative $O(C_F^2\alpha_s^2)$ Darwin corrections amount to -6% to -2% around the $1S$ peak and to -2% to -1% for higher energies. For a more rigorous treatment of the corrections due to the off shellness of the top quark we refer the reader to [29] and references therein.

Although the $O(C_F^2\alpha_s^2)$ Darwin corrections discussed above represent only a small part of the full $O(\alpha_s^2)$ corrections, we believe that their size can be taken as an order of magnitude estimate for the sum of all $O(\alpha_s^2)$ corrections. We therefore have to face the questions of 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 $O(C_F^2\alpha_s^2)$ 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 [14] by using more general arguments that the large top quark mass and width serve as a screening device which protects the $t\bar{t}$ properties in the threshold region from the influence of nonperturbative effects, making the $t\bar{t}$ system 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 $O(C_F^2\alpha_s^2)$ Darwin corrections for the top system are at the

level of a few percent for the most of the threshold region.[20] 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 $O(\alpha_s^2)$ treatment has ever been accomplished there. Further, the theoretical uncertainty of such a complete analysis would then be roughly 1%–2% around the $1S$ peak and below several per mille for higher energies. This can be estimated by taking the α_s values presented below Eq. (45) cubed [assuming that no scales lower than $C_F\alpha_s M_Q$ are relevant for the corrections beyond the $O(\alpha_s^2)$ accuracy level] and by observing the sensitivity of the $O(C_F^2\alpha_s^2)$ 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 $O(\alpha_s^2)$ corrections would be needed, i.e. an $O(\alpha_s^3)$ 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 [32–34] that a proper theoretical description of the bottom system can only be achieved by taking into account nonperturbative corrections, which cannot be calculated analytically from first principles in QCD. On the other hand, it has been demonstrated in [25] that a quite acceptable ''parameter-free'' description of the (S-wave, $l=0$) $b\bar{b}$ bound states with low radial excitation is possible by using perturbative calculations supplemented by nonperturbative 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 formulas including only the effects of the one-loop running of the strong coupling and the global $O(\alpha_s)$ correction factor $(1-4C_F\alpha_s/\pi)$. The question of whether the $O(\alpha_s^2)$ perturbative corrections lead to a still converging series was not addressed explicitly. Equipped with the results for the $O(C_F^2\alpha_s^2)$ 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 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 [35] 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 $O(C_F^2\alpha_s^2)$ 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 II). Here, however, nonperturbative contributions get more and more out of control [33,34] 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 $O(C_F^2\alpha_s^2)$ 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%–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 α_s values given below Eq. (45) 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 $O(C_F^2\alpha_s^2)$ Darwin corrections we used the renormalized Green function at zero distances, Eq. (18), without any further explanation. This is slightly misleading because it implies that the $O(C_F^2\alpha_s^2)$ Darwin corrections to wave functions and cross sections can be uniquely separated from all the other $O(C_F^2\alpha_s^2)$ 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 $O(C_F^2\alpha_s^2)$ 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 Secs. II and III. There, all constants are correct due to proper matching to the well established one- and two-loop expressions $\Pi^{1\,\mathrm{loop}}$ and $\Pi^{2\,\mathrm{loop}}$, Eqs. (8) and (9).

[20] A comparison of the size of the $O(C_F^2\alpha_s^2)$ Darwin corrections with the $O(C_F\alpha_s)$ corrections from the $(1-4C_F\alpha_s/\pi)$ suppression factor is slightly misleading in this context because the latter represents a pure short-distance contribution. Therefore the $O(C_F\alpha_s)$ correction should not be included in a discussion on the convergence in the perturbative description of long-distance corrections. However, for the convenience of the reader, the size of the large $O(C_F\alpha_s)$ corrections shall also be given. It has been shown in [7,30,31] in a two-loop analysis that the scale in the strong coupling of the $O(C_F\alpha_s)$ suppression factor is $e^{-11/24}M_Q$ in the $\overline{\mathrm{MS}}$ scheme. This results in $-4C_F\alpha_s/\pi=-20\%$, -41% and -64% for the top, bottom and charm systems, respectively, using the one-loop QCD beta function, the pole mass values given below Eq. (45) and $\alpha_s(M_z=91.187\ \mathrm{GeV})=0.125$.

V. 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 $O(\alpha^2)$ accuracy, Eq. (19).

We have shown in Sec. III 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. (13)], essentially has to be added to the one- and two-loop expressions for the vacuum polarization function in order to achieve $O(\alpha^2)$ accuracy in the threshold region $|\beta| \lesssim \alpha$. Far from the threshold regime, however, A represents contributions of order α^3 and higher and therefore is irrelevant. This is what we mean by using the term ''valid for all energies to $O(\alpha^2)$ accuracy,'' but not more.

At this point the reader might be tempted to apply formula (19), 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 (19) can be expanded in terms of small q^2. Taking into account only the first nonvanishing contributions in q^2/M^2 and including only contribution up to $O(\alpha^3)$ the result reads

$$\Pi_{\rm QED}^{O(\alpha^2)}(q^2) \stackrel{q^2\to 0}{=} \left(\frac{\alpha}{\pi}\right)\frac{1}{15}\frac{q^2}{M^2}+\left(\frac{\alpha}{\pi}\right)^2\frac{41}{162}\frac{q^2}{M^2} + \alpha^3\frac{\pi^2}{48}\sqrt{\frac{q^2}{M^2}}+O(\alpha^4), \tag{46}$$

where the numerical coefficient of the $O(\alpha^3)$ coefficient is $\pi^2/48=0.21$. The corresponding multiloop expression including also the real first nonvanishing three-loop coefficient (see [4] for details of the three-loop calculation) reads

$$\Pi_{\rm QED}^{3\ \rm loop}(q^2) \stackrel{q^2\to 0}{=} \left(\frac{\alpha}{\pi}\right)\frac{1}{15}\frac{q^2}{M^2}+\left(\frac{\alpha}{\pi}\right)^2\frac{41}{162}\frac{q^2}{M^2} + \left(\frac{\alpha}{\pi}\right)^3\left[-\frac{8687}{13824}+\frac{\pi^2}{3}\left(\frac{1}{8}-\frac{1}{5}\ln 2\right) + \frac{22781}{27648}\zeta_3\right]\frac{q^2}{M^2}+O(\alpha^4). \tag{47}$$

The numerical value of the constant term in the brackets is 0.32. It is evident that the $O(\alpha^3)$ contributions which come from $\Pi_{\rm QED}^{O(\alpha^2)}$ and therefore contain information on the formation of positronium bound states are much larger than the real three-loop contributions. The ratio between the former $O(\alpha^3)$ contributions and the real three-loop result even diverges for $q^2\to 0$. 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. (46) contradict the Appelquist-Carrazone theorem [36] and even represent contributions nonanalytic at $q^2=0$. The solution to this apparent paradox is that $\Pi_{\rm QED}^{O(\alpha^2)}$ only describes the vacuum polarization function to $O(\alpha^2)$ accuracy. All contributions of order α^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 $O(\alpha^2)$ 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 were known for all energies (in the same sense as they are known for the one- and two-loop contributions, $\Pi^{1\ \rm loop}$ and $\Pi^{2\ \rm loop}$). We then could try to determine the expression for the vacuum polarization function valid to $O(\alpha^3)$ accuracy for all energies in the same way as we have determined $\Pi_{\rm QED}^{O(\alpha^2)}$, which is valid to $O(\alpha^2)$ accuracy for all energies. This would be achieved by matching the three-loop expression for the vacuum polarization function to the corresponding $O(\alpha^3)$ formula calculated in NRQED in the same way as presented in Sec. II. The vacuum polarization function valid to $O(\alpha^3)$ accuracy for all energies would then have the form[21]

$$\Pi_{\rm QED}^{O(\alpha^3)}(q^2)=\Pi^{1\ \rm loop}(q^2)+\Pi^{2\ \rm loop}(q^2)+\Pi^{3\ \rm loop}(q^2) + A(\alpha,\beta)-\alpha^3\left[i\frac{\pi^2}{24\beta}\right]+\Delta(\alpha,\beta). \tag{48}$$

In the second line of Eq. (48) the contribution $\alpha^3[i\,\pi^2/24\beta]$ has to be subtracted in order to avoid double counting in the threshold regime since

$$\Pi^{3\ \rm loop}(q^2) \stackrel{|\beta|\ll 1}{=} \alpha^3\left[i\frac{\pi^2}{24\beta}\right]+O(\alpha^3\beta^0). \tag{49}$$

It is therefore clear that far from threshold the second line of Eq. (48) only contains contributions of order α^4 and higher [see Eq. (23)]. Expanding now $\Pi_{\rm QED}^{O(\alpha^3)}$ for small values of q^2 would give a result identical to the three-loop expression, Eq. (47). The large nonanalytical $O(\alpha^3)$ contribution which appeared in Eq. (46) would be gone. It is obvious that this large contribution originates from the leading nonvanishing term of $\Pi^{(3)}$ in an expansion for $|\beta|\ll 1$ evaluated for small q^2. These contributions survive in $\Pi_{\rm QED}^{O(\alpha^2)}$, Eq. (19), but are canceled in $\Pi_{\rm QED}^{O(\alpha^3)}$, Eq. (48). Using the same line of arguments it can easily be shown that all contributions of the function A would be canceled if formulas for the vacuum polarization function with successively higher accuracy would be determined.

[21] In Eq. (48) $\Delta(\alpha,\beta)$ denotes the $O(\alpha^3)$ 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 $O(\alpha^3)$ contributions in Eq. (46). However, it is straightforward to see that Δ contains terms of order α^3 in the threshold regime, but is of order α^4 far from the threshold point.

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 nonrelativistic 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 the function A the greater part of the large corrections will be canceled off, leaving the results which can be obtained from conventional (multiloop) 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 region. There, the contributions of the function A represent unphysical (and gauge noninvariant) contributions which cannot even be used to estimate the size of the real higher-order corrections.[22]

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

$$\mathcal{M}_n(q^2)\equiv\left(\frac{d}{dq^2}\right)^n\Pi(q^2)\sim\int\frac{dq'^2}{q'^2}\frac{\mathrm{Im}\,\Pi(q'^2)}{(q'^2-q^2)^n}. \quad (50)$$

For large n and $|q^2|\ll 4M^2$ 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 α_s and the bottom quark mass from experimental data on the Υ resonances [8]. In this publication it is claimed that $O(\alpha_s^2)$ corrections to the moments $\mathcal{M}_n^{\mathrm{QCD}}(0)$ have been calculated because (conventional) two-loop QCD corrections to the $b\bar{b}$ production cross section have been included in the analysis. It should be clear from the discussions of Sec. IV 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 [8] 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 (see Table 4 in [8]). The latter observation is taken as a ''final test on the importance of higher-order corrections.'' However, as shown in Sec. IV, the $O(\alpha_s^2)$ corrections to the cross section in the threshold region, which contain a resummation of contributions to all orders in the number of loops, are expected to be at the 10%–20% level and will therefore have a large impact on QCD sum rule calculations in the large n limit. The mistake in the arguments of [8] is that it is implicitly assumed that the Sommerfeld factor, Eq. (41), accounts for the resummation of all long-distance effects. Therefore all corrections to expression (41) should be calculable by fixed-order loop calculations alone. This is true for the $O(\alpha_s)$ short-distance correction factor $(1-4C_F\alpha_s/\pi)$, which can be extracted from a pure one-loop calculation, but this is not the case for higher-order corrections like the $O(C_F^2\alpha_s^2)$ Darwin corrections calculated in Sec. IV. 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 [8] it is 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 α_V, which effectively incorporates the short-distance corrections of the QCD potential [40,41], at the scale $M_b\beta$ into the Sommerfeld factor. 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. [See the discussion below Eq. (44).] As a consequence the calculations presented in [8] are not only not at the $O(\alpha_s^2)$ accuracy level but also include a systematic error at order α_s and therefore contain much larger uncertainties than presented there. The authors of [8] finally criticize an older QCD sum rule calculation by Voloshin [7] on the same subject, claiming that in [7] the magnitude of higher-order corrections was underestimated. In this point we agree with the authors of [8] because in [7] it is assumed that $O(\alpha_s^2)$ corrections have ''no enhancement'' in the large n limit. The author of [7] therefore concludes that the entire $O(\alpha_s^2)$ corrections can be parametrized by multiplying the expression containing the leading and next-to-leading $[O(\alpha_s)]$ effects for $\mathcal{M}_n^{\mathrm{QCD}}(0)$ [see Eqs. (6), (11) and (24) of [7], respectively] with the global factor $(1+c/n)$, where the constant c has to be determined from fitting the resulting formula to the Υ family data. The results of the fitting procedure are $\alpha_s(M_z)=0.109\pm 0.001$, $M_b=4827\pm 7$ MeV and $c=-0.59\pm 0.19$, where M_b is the bottom quark pole mass and α_s is the strong coupling in the $\overline{\mathrm{MS}}$ scheme. The errors quoted in [7] for $\alpha_s(M_z)$ and M_b were derived by a combination of the statistical errors with the difference in the central values by performing the fits, taking $c=0$ and leaving c as a fit parameter. The error in c is statistical. The reason for the small errors [$\delta M_b/M_b=0.1\%$ and $\delta\alpha_s(M_z)/\alpha_s(M_z)=1\%$] is the strong dependence of the fitting formula [Eq. (24) of [7]] on the parameters α_s (through terms proportional to $(\alpha_s\sqrt{n})^3$ and $\exp[(\alpha_s\sqrt{n})^2]$) and M_b (through a term proportional to M_b^{2n}) and the assumptions that all $O(\alpha_s^2)$ corrections can be parametrized in form of the global factor $(1+c/n)$, where c

[22] If applied to QCD our conclusion is essentially equivalent to arguments employed in [37,38] where the large effects of the $t\bar{t}$ threshold on electroweak parameters proposed in [39] have been criticized.

is of order one. In the following we give some arguments why the latter assumption is wrong and why the real errors in the values of $\alpha_s(M_z)$ and M_b are much bigger than claimed in [7]: (i) In [7] the range $8 \leqslant n \leqslant 20$ is considered. According to the fitted value for c this would correspond to relative $O(\alpha_s^2)$ corrections of about 10% and 5% for $n=8$ and 20, respectively, which shows that in [7] $O(\alpha_s^2)$ corrections become smaller when the value of n is increased. Because the QCD sum rules are more and more sensitive to the $(J^{PC}=1^{--})$ $b\overline{b}$ ground state for larger values of n, this would implicitly mean that the $O(\alpha_s^2)$ corrections to the $b\overline{b}$ ground state $[\Upsilon(1S)]$ would be extremely small. We have explicitly shown 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%–20% for the modulus squared of the ground state wave function at the origin for a bound $b\overline{b}$ pair and are far from being small. We therefore conclude that the $O(\alpha_s^2)$ corrections to the formulas presented in [7] cannot be parametrized in terms of a global factor with the form $(1+c/n)$. (ii) In [7] the $O(\alpha_s)$ corrections induced by the running of the strong coupling have been included by taking into account the logarithmic terms in the QCD potential [40,41] using time-independent perturbation theory. This determines the effective scale of the strong coupling in the leading order contributions to $\mathcal{M}_n^{\mathrm{QCD}}(0)$. However, because the $O(\alpha_s^2)$ corrections from the running of the strong coupling have not been taken into account, there is still a relative error of order α_s in the actual value of this scale. Therefore, although the value of α_s can be determined with high accuracy in the fitting process, the actual value of the scale of α_s is still subject to higher order uncertainties.[23] It can be easily checked that this uncertainty results in a relative error of order $\delta\alpha_s(M_z)/\alpha_s(M_z) \sim \alpha_s(M_z) \sim 10\%$ for the value of the strong coupling at the scale M_z. (iii) Because in [7] only $O(\alpha_s)$ corrections are included, the masses of the $b\overline{b}$ bound states (i.e. their bound state energies) are only taken into account up to order α_s^3. $O(\alpha_s^4)$ contributions to the bound state masses [corresponding to the $O(\alpha_s^2)$ corrections to the leading order expressions for $\mathcal{M}_n^{\mathrm{QCD}}(0)$] have not been taken into account. It can be easily seen that those $O(\alpha_s^4)$ contributions to the bound state masses would cause the fitting formula to depend on $[M_b + \text{terms of order } O(\alpha_s^4)]^{2n}$ rather than just M_b^{2n}. As a consequence the value of M_b extracted in [7] really contains a relative error of order[24] $\delta M_b/M_b \sim \alpha_s^4 \sim 0.5\%-2\%$. Taking into account the arguments (i)–(iii) we have to conclude that the real (theoretical) uncertainties of the $\alpha_s(M_Z)$ and M_b values presented in [7] are about an order of magnitude larger than claimed there. Only a complete determination of all $O(\alpha_s^2)$ corrections to $\mathcal{M}_n^{\mathrm{QCD}}(0)$ will lead to a reduction of these uncertainties.

VI. SUMMARY

In this work we have used the concept of effective field theories to calculate the $O(\alpha^2)$ contributions to the QED vacuum polarization function in the threshold region and to define a renormalized (i.e. finite) version of the zero-distance Coulomb Green function which can be used for higher order calculations in textbook quantum mechanics time-independent perturbation theory. In the framework where nonrelativistic 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 employing textbook 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 multiloop techniques (in conventional covariant perturbation theory) have to be employed. We have demonstrated that the approach employed in this work represents an efficient method to merge sophisticated multiloop 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 systematic separation of long- and short-distance physics at any level of precision. For our calculations we have used the ''direct matching'' procedure which can be applied if the multiloop results to the quantity of interest are at hand. The direct matching allows for a quite sloppy treatment of UV divergences in the effective field theory and, therefore, can be carried out with much less effort compared to the conventional matching procedure. However, the direct matching is of no value if quantities shall be calculated for which no multiloop expressions are available.

We have demonstrated the efficiency of our approach by calculating the $O(\alpha^6)$ vacuum polarization effects in the single photon annihilation contributions to the positronium ground state hyperfine splitting without referring back to the Bethe-Salpeter equation. We found an error in an older calculation on the same subject. We have determined 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 $t\overline{t}$ 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 $b\overline{b}$ 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 $c\overline{c}$ 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

[23] In [7] the value of the strong coupling at the scale of order 1 GeV was determined as $\alpha_s(1\ \mathrm{GeV}) = 0.336 \pm 0.011$. However, the scale 1 GeV is subject to unknown higher order corrections of order $\alpha_s(1\ \mathrm{GeV}) \approx 30\%$ itself, i.e. $\alpha_s(1 \pm 0.3\ \mathrm{GeV}) = 0.336 \pm 0.011$.

[24] The scale of the strong coupling in the perturbative series for the bound state masses is of order $M_b\alpha_s$ rather than M_b. We therefore have used the range of values $\alpha_s(C_F\alpha_s M_b) = 0.25-0.38$ presented below Eq. (45) for our estimate of $\delta M_b/M_b$.

governing the $O(\alpha_s^2)$ corrections. 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 and the resulting bad convergence of the corresponding perturbative series.

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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