All-Order Binding Corrections to Muonium Hyperfine Splitting

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The use of exact Dirac-Coulomb propagators allows the evaluation of binding corrections to the Schwinger correction in ground state muonium hyperfine splitting to all orders. The calculational method is described and the results are used firstly to verify recent perturbative calculations of higher-order binding corrections and secondly to evaluate the residual terms of still higher order. Implications for muonium hyperfine splitting are discussed. [S0031-9007(97)03490-X]

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Calculations of radiative corrections in atomic physics are frequently expressed in terms of a double expansion in the fine structure constant α and the quantity $Z\alpha$, where Z is the nuclear charge. This is done even when $Z = 1$, as it serves to distinguish purely radiative effects from *binding corrections,* which are effects arising from the expansion of the Dirac-Coulomb propagator in terms of interactions with the nuclear Coulomb potential. In atomic physics, these binding corrections can have large coefficients, which has two consequences. One is that at high Z, these large coefficients now multiply the no longer small quantity $Z\alpha$, and a complete breakdown of the series may result, in the sense that the value of the series terminated at a given order can change in sign and order of magnitude when the next order is included. For highly charged ions there is no substitute for a nonperturbative evaluation to all orders in $Z\alpha$. The second is that even at $Z = 1$, adequate comparison with high-accuracy experiments can require relatively high orders of perturbation theory to be considered. Given that the already quite precisely determined hyperfine splitting of the ground state of muonium [1],

$$\Delta\nu_{\rm exp} = 4\,463\,302.88(16)\ \text{kHz}\,, \tag{1}$$

is in the process of being even more accurately measured [2], a complete treatment of these high-order terms has become an important problem for QED theory.

It is convenient to define a set of functions $D^{(2n)}(Z\alpha)$ that parametrize radiative corrections to the ground-state hyperfine splitting. Specifically, in the nonrecoil, point-nucleus limit, radiative corrections to muonium hyperfine splitting can be written as

$$\Delta\nu = E_F(1 + a_\mu)\left[\frac{1}{\gamma(2\gamma - 1)} + \frac{\alpha}{\pi}D^{(2)}(Z\alpha) + \left(\frac{\alpha}{\pi}\right)^2 D^{(4)}(Z\alpha) + \cdots\right], \tag{2}$$

where

$$E_F = \frac{16}{3}Z^3\alpha^2 cR_\infty \frac{m_e}{m_\mu}\left(1 + \frac{m_e}{m_\mu}\right)^{-3}, \tag{3}$$

$\gamma = \sqrt{1 - (Z\alpha)^2}$, and a_μ is the muon anomalous magnetic moment. Note that we have chosen to exclude the full magnetic moment of the muon in our definition of E_F, since while the factor $1 + a_\mu$ is always present for nonrecoil corrections, it is not naturally present for recoil corrections, which we will include later. The functions $D^{(2n)}(Z\alpha)$ generalize the n-loop expansion of the electron $g - 2$ factor. In particular, the self-energy part of $D^{(2)}(Z\alpha)$ is given by

$$D^{(2)}_{\rm SE}(Z\alpha) = \frac{1}{2} + \left(\ln 2 - \frac{13}{4}\right)\pi(Z\alpha) + \left[-\frac{8}{3}\ln^2(Z\alpha) + \left(-\frac{37}{36} + \frac{16}{3}\ln 2\right) \times \ln(Z\alpha) + E^{(2)}_{\rm SE}(Z\alpha)\right](Z\alpha)^2, \tag{4}$$

where we introduce the function $E^{(2)}_{\rm SE}(Z\alpha)$ that includes the constant that enters in order $(Z\alpha)^2$ along with all higher order terms. Recent calculations [3–5] allow the further reparametrization

$$E^{(2)}_{\rm SE}(Z\alpha) = 17.122 + \left[\left(-5\ln 2 + \frac{191}{16}\right)\pi\ln(Z\alpha) + F^{(2)}_{\rm SE}(Z\alpha)\right](Z\alpha)\,, \tag{5}$$

where the function $F^{(2)}_{\rm SE}(Z\alpha)$ contains the unknown constant that enters in order $(Z\alpha)^3$ plus all higher-order corrections.

The function $D^{(2)}_{\rm SE}(Z\alpha)$, which has been evaluated to all orders in $Z\alpha$ for a range of Z in Refs. [6,7], is strongly Z

dependent: while it tends to the Schwinger value of $1/2$ in the limit $Z \rightarrow 0$, it changes sign already at $Z = 8$, and becomes (in units in which the finite size of the nucleus and the Breit correction are built into E_F) -3.86 and -5.14 at the experimentally interesting cases of $Z = 67$ [8] and $Z = 83$ [9], respectively. These values differ in sign and in order of magnitude from the perturbative expression.

While an exact approach is essential for high Z, it is also useful for low Z. This is because a nonperturbative approach automatically includes all the corrections listed above in Eqs. (4) and (5) along with all higher-order corrections. Given that $E_{\rm SE}^{(2)}$ is effectively changed from the constant 17.122 to a value of 16.166 by the next-order logarithmic term at $Z = 1$, it is important to account for the remaining terms of $E_{\rm SE}^{(2)}$. In particular, a large constant in order $Z\alpha$ and high powers of $\ln(Z\alpha)$ in order $(Z\alpha)^2$ are to be expected and must be accounted for. The calculations described below show that the net effect of these terms is, in fact, relatively small. They do, however, provide confirmation of the recently determined constant and the logarithmic term in Eq. (5), and allow a determination of the higher-order terms with a precision well under the experimental error [1].

While in this Letter we will be concerned only with the self-energy term, we note for completeness that the vacuum polarization term is

$$D_{\rm VP}^{(2)}(Z\alpha) = \frac{3}{4}\,\pi(Z\alpha) + \left[-\frac{8}{15}\ln(Z\alpha) + E_{\rm VP}^{(2)}(Z\alpha)\right] \times (Z\alpha)^2, \quad (6)$$

where the first term in $E_{\rm VP}^{(2)}$ has recently been recalculated [4,10] and determined to be $-\frac{8}{15}\ln 2 + \frac{34}{225} = -0.218\,567$. The coefficient of the logarithmic term of the next order has also been calculated to be $-13\pi/24$ [5]. Remaining higher-order corrections should be quite unimportant.

The starting point of our calculation of $D_{\rm SE}^{(2)}(Z\alpha)$ is the standard formula for the self-energy shift of a bound electron,

$$\Delta E = -ie^2 \int d^3x \int d^3y \int \frac{d^4k}{(2\pi)^4} \frac{\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})]}{k^2 + i\delta} \times \bar{\psi}_v(\mathbf{x})\gamma_\mu S_F(\mathbf{x},\mathbf{y};\epsilon_v - k_0)\gamma^\mu \psi_v(\mathbf{y}). \quad (7)$$

If a nuclear magnetic-dipole field is present in addition to the nuclear Coulomb field, the wave functions, electron propagator, and the energy ϵ_v in Eq. (7) are all modified, and each modification gives rise to a different contribution to the hyperfine structure. The wave function modification term, denoted E_S^A in the following, is evaluated using numerical techniques developed for the self-energy problem [11], with one of the wave functions replaced by a wave function modified by the magnetic-dipole field. The modification of the electron propagator leads to a term we refer to as the vertex term E_V, and the modification of the energy to a term we refer to as the derivative term E_S. The latter two terms have canceling ultraviolet divergences. To evaluate them, we first subtract terms in which the bound propagators are replaced with free propagators, terms which we refer to as E_S^p and E_V^p. The differences $E_S^s = E_S - E_S^p$ and $E_V^s = E_V - E_V^p$, which are ultraviolet convergent, are then evaluated in configuration space. It remains to add back the finite parts of E_S^p and E_V^p; these are extracted by dimensional regularization and evaluated in momentum space. The divergent parts of E_S^p and E_V^p cancel as a consequence of the Ward identity. The various contributions to the hyperfine structure are tabulated in Table I.

A complication of the calculation is the presence of certain singularities in the ultraviolet-finite subtracted terms, E_S^s and E_V^s, that occur when intermediate states in the spectral representation of the internal propagators are degenerate with the valence state. These singularities cancel in the sum $E_S^s + E_V^s$, and for this reason we tabulate that sum in the fourth column of Table I. It is regulated by replacing ϵ_v with $\epsilon_v(1-\delta)$. While both E_S^s and E_V^s diverge logarithmically with δ, their sum has a smooth limit as $\delta \rightarrow 0$.

Table I differs from a related table presented in our previous work [7] in three ways. First, the Fermi splitting in the previous paper was taken to include relativistic corrections, and in the present case it is not; thus there is a difference of normalization. Second, because of their relatively large effect at high Z, finite-nuclear-size effects were included in [7], while here, because we are interested in making predictions for muonium, the point-Coulomb limit was taken for all Z. Finally, and most importantly, we have increased the accuracy of the previous calculation, because the previous values were not precise enough to make a reliable determination of $D_{\rm SE}^{(2)}(1\alpha)$ needed to infer the muonium hyperfine splitting.

Several issues had to be addressed to reach an accuracy of 1×10^{-5} claimed in the present calculation for $Z = 3$–25, of 2×10^{-5} for $Z = 2$, and of 3×10^{-5}

TABLE I. Contributions to $D_{\rm SE}^{(2)}(Z\alpha)$.

Z	E_S^A	$E_S^p + E_V^p$	$E_V^s + E_S^s$	Total
1	−0.010 97	2.709 98	−2.260 93	0.438 08(3)
2	−0.029 32	2.596 75	−2.193 96	0.373 47(2)
3	−0.051 86	2.491 24	−2.131 79	0.307 59(1)
4	−0.077 30	2.392 20	−2.073 87	0.241 03(1)
5	−0.104 95	2.298 75	−2.019 76	0.174 05(1)
6	−0.134 32	2.210 25	−1.969 09	0.106 84(1)
7	−0.165 10	2.126 16	−1.921 56	0.039 50(1)
8	−0.197 06	2.046 07	−1.876 91	−0.027 91(1)
9	−0.230 03	1.969 60	−1.834 92	−0.095 35(1)
10	−0.263 89	1.896 44	−1.795 38	−0.162 83(1)
15	−0.443 86	1.571 84	−1.629 02	−0.501 03(1)
20	−0.638 80	1.299 59	−1.504 35	−0.843 56(1)
25	−0.848 84	1.064 06	−1.411 44	−1.196 21(1)

for $Z = 1$. First, E_S^p and E_V^p behave asymptotically as $E_S^p = -2\ \ln(2Z\alpha) - \frac{2}{3}$ and $E_V^p = 2\ \ln(2Z\alpha) + \frac{7}{2}$. By subtracting out these large terms, remaining integrations could be controlled to well under 10^{-5}. Most of the other terms are treated in coordinate space, with the photon propagator expanded in a partial-wave expansion. Because the partial-wave sum cannot be extended to infinity, it is necessary to work to sufficiently high L values that a clear asymptotic behavior is found. At the lowest Z this required going to values of about $L = 50$ in both $E_S^s + E_V^s$ and the part of E_S^A that is carried out in coordinate space. Our estimated errors are dominated by the numerical uncertainty in these partial-wave extrapolations, as well as the uncertainty in the part of E_S^A evaluated in momentum space, which is significantly more difficult to control than the corresponding term in the Lamb shift calculation.

We carry out our analysis of the data in Table I in two parts. In the first, we fit $E_{\rm SE}^{(2)}(Z\alpha)$, which is tabulated in Table II, to the form given in Eq. (5), but with undetermined coefficients. This is meant to provide a check of the consistency of the recent calculations with our method. The fits are relatively insensitive to the form chosen for $F_{\rm SE}^{(2)}(Z\alpha)$, and a typical fit yields 17.2(1) for the constant and $-26.5(2.0)$ for the coefficient of the logarithmic term, which analytically is -26.615. Here and later, errors quoted for fits reflect the sensitivity of the fit to the higher-order terms included, in particular, to logarithmic terms in order $(Z\alpha)^4$ in $D^{(2)}(Z\alpha)$.

In the next part of the analysis we assume the correctness of the constant and logarithmic terms in Eq. (5), and evaluate $F_{\rm SE}^{(2)}(Z\alpha)$, which is tabulated in Table II. Even before doing any fitting, we note the fact that $F_{\rm SE}^{(2)}(Z\alpha)$ varies smoothly in the range $3 \le Z \le 25$ (towards about -12 at $Z = 1$) is again a confirmation that the first two terms of Eq. (5) have been correctly incorporated into our all-order calculation. We also find our most important conclusion, namely, that the sum of all higher-order terms is very small, contributing approximately -0.09 to $E_{\rm SE}^{(2)}(1\alpha)$. A detailed fit gives the sum of all previously uncalculated terms to be

$$F_{\rm SE}^{(2)}(1\alpha) = -12.0(2.0)\,, \tag{8}$$

which, taken together with the other terms in Eq. (5), gives the main result of this Letter,

$$E_{\rm SE}^{(2)}(1\alpha) = 16.079(15)\,. \tag{9}$$

The error corresponds to an uncertainty of 0.008 kHz for muonium ground-state hyperfine splitting.

We note that if we fit directly to $E_{\rm SE}^{(2)}(Z\alpha)$ in Table II, without necessarily assuming the correctness of the first two terms in Eq. (5), we infer $E_{\rm SE}^{(2)}(1\alpha) = 16.10(5)$, a value consistent with (9), though less accurate. We note also that there are some discrepancies between our present results and those given in Ref. [6]. Specifically, our results of 0.438 08, 0.307 59, 0.174 05, 0.039 50, and $-0.162\,83$ for $D_{\rm SE}^{(2)}(Z\alpha)$ at $Z = 1$, 3, 5, 7, and 10, respectively, disagree in the third or fourth digit with the quoted results of 0.4379, 0.3072, 0.1733, 0.0366, and -0.1640 from that work. These discrepancies can lead to very different inferred values of higher-order corrections to $E_{\rm SE}^{(2)}(1\alpha)$.

Before discussing the comparison with experiment, we mention that our total result for $E_{\rm SE}^{(2)}(1\alpha)$ above differs from an earlier calculation [12] that found $E_{\rm SE}^{(2)}(1\alpha) = 15.1(3)$. However, the previous calculation, while similar to the present one in that some terms were evaluated to all orders in $Z\alpha$, was based on a perturbative expansion of the Dirac-Coulomb Green's function in terms of a relativistic generalization of the nonrelativistic Coulomb Green's function. Terms that explicitly started in order $(Z\alpha)^3$ were not treated, though some such terms were included if they were part of expressions that entered in a lower order. Because the portion of the relatively large higher-order terms included in the previous calculation has not been determined, the results are not necessarily discrepant. However, the present calculation is meant to supplant that work.

Now that $E_{\rm SE}^{(2)}(1\alpha)$ is very accurately known, a theoretical prediction can be made for ground-state muonium hyperfine splitting. If we use the value of α inferred from the electron anomalous magnetic moment $\alpha^{-1} = 137.035\,999\,93(52)$ [13] and $m_\mu/m_e = 206.768\,262(62)$ [1,14], then E_F is

$$E_F = 4\,453\,839.38(1.33)\,(0.03)\ \text{kHz}\,. \tag{10}$$

A principal aim of the new experiment [2] is the reduction of the first error, which arises from the uncertainty of the muon mass. To complete the nonrecoil corrections, we note that the function $D^{(4)}(Z\alpha)$ has been determined to be [15–17]

$$D^{(4)}(Z\alpha) = a_e^{(4)} + [0.7717(4)]\pi(Z\alpha) + \left[-\frac{4}{3}\ \ln^2(Z\alpha)\right](Z\alpha)^2. \tag{11}$$

TABLE II. Contributions to $E_{\rm SE}^{(2)}(Z\alpha)$ and $F_{\rm SE}^{(2)}(Z\alpha)$.

Z	$E_{\rm SE}^{(2)}(Z\alpha)$	$F_{\rm SE}^{(2)}(Z\alpha)$
1	15.66(56)	−70(77)
2	15.29(9)	−12.7(6.4)
3	14.60(2)	−13.64(95)
4	13.97(1)	−13.85(40)
5	13.379(8)	−14.46(21)
6	12.823(5)	−14.92(12)
7	12.298(4)	−15.283(75)
8	11.798(3)	−15.584(50)
9	11.321(2)	−15.856(35)
10	10.862(2)	−16.113(26)
15	8.7901(8)	−17.240(8)
20	6.9746(5)	−18.307(3)
25	5.3255(3)	−19.380(2)

Nonleading log terms in order $(Z\alpha)^2$ have been considered [13], and are estimated to contribute -0.110 kHz. No binding corrections to higher-order $D^{(n)}(Z\alpha)$ functions have been calculated, so these are replaced with a_e^n. The dominant recoil corrections are [18]

$$\Delta\nu_{\text{recoil}} = E_F\Big\{-\frac{3Z\alpha}{\pi}\frac{m_e m_\mu}{m_\mu^2 - m_e^2}\ln\frac{m_\mu}{m_e} + \frac{(Z\alpha)^2 m_r^2}{m_e m_\mu}\Big[-2\ln(Z\alpha) - 8\ln 2 + \frac{65}{18}\Big] + \frac{\alpha(Z\alpha)}{\pi^2}\frac{m_e}{m_\mu} \times\Big[-2\ln^2\frac{m_\mu}{m_e} + \frac{13}{12}\ln\frac{m_\mu}{m_e} + \frac{21}{2}\zeta(3) + \zeta(2) + \frac{35}{9} + 2.15(14) + \frac{\alpha}{\pi}\Big(-\frac{4}{3}\ln^3\frac{m_\mu}{m_e} + \frac{4}{3}\ln^2\frac{m_\mu}{m_e}\Big) + \frac{8\pi Z\alpha}{3}\ln^2(Z\alpha)\Big(2 - \frac{Z}{4}\Big)\Big] + \frac{3(Z\alpha)^3}{\pi}\frac{m_e}{m_\mu}\ln\frac{m_\mu}{m_e}\ln Z\alpha\Big\}. \quad (12)$$

In addition to the above, higher-order recoil corrections of order $(Z\alpha)^3 m_e/m_\mu \ln Z\alpha$ have been estimated as -151 kHz [13]. Including these terms along with the weak interaction contribution of -0.065 kHz, the present theoretical prediction is

$$\Delta\nu_{\text{theory}} = 4\,463\,302.89(1.33)\,(0.03)\ \text{kHz}. \quad (13)$$

Now that the principal uncertainty associated with the nonrecoil part of the calculation has been essentially eliminated, the completion of the remaining recoil corrections that contribute at this level together with results from the new experiment will allow a significantly more stringent test of QED to be obtained from muonium hyperfine splitting.

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