

Order $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$ Corrections to the $n=1$ and $n=2$ Energy Levels of Positronium

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The order $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$ corrections to the $n=1$ and $n=2$ energy levels of positronium are calculated using the conventional Bethe-Salpeter formalism. The Barbieri-Remiddi potential provides a suitable zeroth-order kernel about which perturbation theory is developed. A simple algorithmic method which amounts to an expansion of the interaction kernel in powers of the momentum divided by the mass is shown to suffice to extract the $\ln \alpha^{-1}$ terms from most of the interaction terms.

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Positronium (Ps) [1-3], the purely leptonic bound state of an electron and positron, is a fertile area of theoretical and experimental research since the investigation of its properties allows for a very accurate test of quantum electrodynamics, a test which is unobscured by the presence of other forces.

The expression for the energy of any positronium state can be written as an ascending series in the fine-structure constant α [4], specifically,

$$\frac{E(n^{2S+1}L_{2J+1})}{h} = f_{\text{RYD}}(a + b\alpha^2 + c\alpha^3 + d\alpha^3 \ln \alpha^{-1} + e\alpha^4 \ln \alpha^{-1} + f\alpha^4 + \dots), \quad (1)$$

where the spectroscopic notation $n^{2S+1}L_{2J+1}$ labels the state and the dependence of the constants a, b, \dots on the quantum numbers n, j, l , and s is suppressed. The Rydberg unit of frequency f_{RYD} is cR_∞ , where R_∞ is the Rydberg wave-number constant [5].

Of primary interest are differences between energy levels. In particular, the energy difference between the two $n=1$ states (the hyperfine splitting), the splitting between the triplet $2S-1S$ states, and the splittings between the $n=2$ triplet $l=0$ state and the $n=2$ triplet $l=1$ states have been the subjects of ongoing experimental research. Consequently, their theoretical values are of significant interest.

For the $n=1$ and $n=2$ states, the constants a, b, c , and d have been calculated [6-11]. The spin-dependent part of e and some of the spin-dependent part of f have been computed for the $n=1$ state (for the hyperfine splitting) [12-20]. In this paper we report on a calculation of the complete coefficient e . This calculation is important as a more precise experiment to measure the $1S-2S$ splitting is planned [21]. This experiment will test theory at the $\alpha^4 f_{\text{RYD}}$ level and so will provide another precision test of QED.

To do the calculation the conventional Bethe-Salpeter equation is employed [22]. The Barbieri-Remiddi solution [19] is used as a solvable zeroth-order equation about which a perturbation series [20] is developed. A typical term in the perturbation series which contributes to the shift of the n th energy level is of the form $\int d^4q d^4p$

$\times \bar{\psi}(p)K(p,q)\psi(q)$, where $\psi(p)$ is the four-dimensional solution to the Bethe-Salpeter equation with the Barbieri-Remiddi kernel, a solution which reduces to the Schrödinger-Coulomb wave functions in the nonrelativistic limit. $K(p,q)$ is an expression which can be associated with the Feynman diagrams. The perturbation series produces integrals which have a complicated functional dependence on α . Aside from the explicit α dependence generated by the number of photons exchanged in a particular Feynman graph, the dependence on the fine-structure constant comes from two main sources (m_e is the electron mass): (1) The functional dependence of the wave functions on the Bohr momentum ($\sim am_e$); and (2) the dependence of any propagators in the kernel $K(p,q)$ on the total energy since this quantity goes as $2m_e + O(m_e \alpha^2)$.

The integrals encountered are in general very complicated and cannot be done exactly. However, in order to calculate the $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$ dependence we can replace the exact integrands by approximate ones which can be integrated and which will reproduce the correct logarithmic behavior. This is because the logarithmic dependence on α can only develop when the integration variables are restricted to the range $\sim am_e$ to m_e . (The variables of integration are the internal momenta.) It suffices then to expand the integrands in powers of the momentum divided by the mass (the nonrelativistic expansion) provided a cutoff of the order of the electron mass is supplied. Then, those terms which in the final momentum integration go as $\int_{\sim am_e}^{m_e} dp (1/p)$ are those which generate $\ln \alpha^{-1}$ expressions and are of interest to this calculation. (This method has been successfully used by others to extract similar expressions for the positronium hyperfine splitting. See in particular Refs. [14] and [20].)

To order $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$, integrals to four loops must be evaluated where each wave-function integration is counted as a loop integration. This requires the computation of terms in the perturbation kernel to two loops. For this calculation it is convenient to use the Coulomb gauge and we find that with the exception of the one transverse photon kernel and those kernels where a transverse photon crosses a Coulomb photon or two parallel Coulomb photons, the expansion of the integrand in powers of momen-

tum over the mass works well. However, for the above-mentioned kernels such a naive expansion does not succeed since spurious infrared divergences are generated. This is a consequence of the more singular nature of these graphs in the low momentum region. This more complicated behavior is first manifested at the $\alpha^3 f_{\text{RYD}}$ level where these graphs contribute to the Bethe logarithm [23].

To calculate the terms of interest of these kernels the leading-order $\alpha^3 f_{\text{RYD}}$ terms are first subtracted, a meth-

od suggested by the work of Grotch and Yennie [24]. Then, nonsingular nonrelativistic expansions can be made on the remainder terms which are sufficient to extract the $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$ terms.

For the $n=1$ state the total $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$ term is 8 times the $n=2$ value. This relation, confirmed by explicit calculation, is a consequence of the same asymptotic form modulo normalizations for all $l=0$ Schrödinger-Coulomb wave functions in the logarithmic region.

Calculations yield the following additions to the energy levels:

$$\begin{aligned} \frac{\Delta E(1^1S_0)}{h} &= [-\frac{1}{4} \alpha^4 \ln \alpha^{-1}] f_{\text{RYD}}, & \frac{\Delta E(1^3S_1)}{h} &= [\frac{1}{6} \alpha^4 \ln \alpha^{-1}] f_{\text{RYD}}, \\ \frac{\Delta E(2^1S_0)}{h} &= [-\frac{1}{32} \alpha^4 \ln \alpha^{-1}] f_{\text{RYD}}, & \frac{\Delta E(2^3S_1)}{h} &= [\frac{1}{48} \alpha^4 \ln \alpha^{-1}] f_{\text{RYD}}, \\ \frac{\Delta E(2^1P_1)}{h} &= [0 \alpha^4 \ln \alpha^{-1}] f_{\text{RYD}}, & \frac{\Delta E(2^3P_2)}{h} &= [0 \alpha^4 \ln \alpha^{-1}] f_{\text{RYD}}, \\ \frac{\Delta E(2^3P_1)}{h} &= [0 \alpha^4 \ln \alpha^{-1}] f_{\text{RYD}}, & \frac{\Delta E(2^3P_0)}{h} &= [0 \alpha^4 \ln \alpha^{-1}] f_{\text{RYD}}. \end{aligned} \quad (2)$$

These values must be added to the $\alpha^2 f_{\text{RYD}}$ and $\alpha^3 f_{\text{RYD}}$ terms. The order $\alpha^2 f_{\text{RYD}}$ terms can be calculated using Ferrell's formula [9]:

$$\frac{\Delta E(nl_s, \alpha^2 f_{\text{RYD}})}{h} = \frac{2\alpha^2 f_{\text{RYD}}}{n^3} \left[\frac{11}{64} \frac{1}{n} - \frac{1}{2(2l+1)} + \frac{7}{12} \delta_{1s} \delta_{0l} + \frac{\delta_{1s}(1-\delta_{0l})}{8(1+\frac{1}{2})} \right] \times \begin{cases} \frac{3l+4}{(l+1)(2l+3)}, & j=l+1, \\ -\frac{1}{l(l+1)}, & j=1, \\ -\frac{(3l-1)}{l(2l-1)}, & j=l-1, \end{cases} \quad (3)$$

while for the $n=2$ states the $\alpha^3 f_{\text{RYD}}$ terms were reported some time ago by Fulton and Martin [10]. However, the $n=1$ terms must be computed separately since terms of this order do not scale as $1/n^3$ as erroneously reported [25]. The correct value has been noted by several groups [26,27].

We can now write down the theoretical expressions for the energy levels and differences of the energy levels of experimental interest:

$$\frac{E(1^3S_1)}{h} = f_{\text{RYD}} \left[-\frac{1}{2} + \frac{49}{96} \alpha^2 + \frac{\alpha^3}{\pi} \left[-\frac{1}{15} + \frac{4}{3} \ln 2 + \frac{3}{2} \ln \alpha^{-1} - \frac{4}{3} \ln R(1,0) \right] + \frac{1}{6} \alpha^4 \ln \alpha^{-1} \right], \quad (4)$$

$$\frac{E(2^3S_1)}{h} = f_{\text{RYD}} \left[-\frac{1}{8} + \frac{65}{1536} \alpha^2 + \frac{\alpha^3}{\pi} \left[\frac{97}{960} + \frac{1}{48} \ln 2 + \frac{3}{16} \ln \alpha^{-1} - \frac{1}{6} \ln R(2,0) \right] + \frac{1}{48} \alpha^4 \ln \alpha^{-1} \right], \quad (5)$$

$$\frac{E(2^3P_2)}{h} = f_{\text{RYD}} \left[-\frac{1}{8} - \frac{43}{7680} \alpha^2 - \frac{\alpha^3}{\pi} \left[\frac{1}{360} + \frac{1}{6} \ln R(2,1) \right] \right], \quad (6)$$

$$\frac{E(2^3P_1)}{h} = f_{\text{RYD}} \left[-\frac{1}{8} - \frac{47}{1536} \alpha^2 - \frac{\alpha^3}{\pi} \left[\frac{5}{288} + \frac{1}{6} \ln R(2,1) \right] \right], \quad (7)$$

$$\frac{E(2^3P_0)}{h} = f_{\text{RYD}} \left[-\frac{1}{8} - \frac{95}{1536} \alpha^2 - \frac{\alpha^3}{\pi} \left[\frac{25}{576} + \frac{1}{6} \ln R(2,1) \right] \right], \quad (8)$$

$$\begin{aligned} v_{21} &= \frac{E(2^3S_1) - E(1^3S_1)}{h} \\ &= f_{\text{RYD}} \left[\frac{3}{8} - \frac{719}{1536} \alpha^2 + \frac{\alpha^3}{\pi} \left[\frac{161}{960} - \frac{21}{16} \ln 2 - \frac{21}{16} \ln \alpha^{-1} - \frac{1}{6} \ln R(2,0) + \frac{4}{3} \ln R(1,0) \right] - \frac{7}{48} \alpha^4 \ln \alpha^{-1} \right], \end{aligned} \quad (9)$$

TABLE I. Numerical values in megahertz of the individual terms in Eqs. (4)–(8). The last two columns are the sums of the terms to order $\alpha^3 f_{\text{RYD}}$ and $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$.

	f_{RYD}	$\alpha^2 f_{\text{RYD}}$	$\alpha^3 f_{\text{RYD}}$	$\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$	Total($\alpha^3 f_{\text{RYD}}$)	Total
$E(1^3S_1)$	-1 644 920 980.55	894 19.17	1 733.14	7.65	-1 644 829 828.24	-1 644 829 820.59
$E(2^3S_1)$	-411 230 245.14	7 413.59	231.71	0.96	-411 222 599.85	-411 222 598.90
$E(2^3P_2)$	-41 130 245.14	-980.87	0.91	0.00	-41 131 225.11	-41 131 225.11
$E(2^3P_1)$	-411 230 245.14	-5 360.59	-5.03	0.0	-411 235 610.75	-411 235 610.75
$E(2^3P_0)$	-411 230 245.14	-10 835.23	-15.63	0.00	-411 241 095.99	-411 241 095.99

$$v_2 = \frac{E(2^3S_1) - E(2^3P_2)}{h} = f_{\text{RYD}} \left[\frac{23}{480} \alpha^2 + \frac{\alpha^3}{\pi} \left(\frac{299}{2880} + \frac{1}{48} \ln 2 + \frac{3}{16} \ln \alpha^{-1} - \frac{1}{6} \ln R(2,0) + \frac{1}{6} \ln R(2,1) \right) + \frac{1}{48} \alpha^4 \ln \alpha^{-1} \right], \quad (10)$$

$$v_1 = \frac{E(2^3S_1) - E(2^3P_1)}{h} = f_{\text{RYD}} \left[\frac{7}{96} \alpha^2 + \frac{\alpha^3}{\pi} \left(\frac{341}{2880} + \frac{1}{48} \ln 2 + \frac{3}{16} \ln \alpha^{-1} - \frac{1}{6} \ln R(2,0) + \frac{1}{6} \ln R(2,1) \right) + \frac{1}{48} \alpha^4 \ln \alpha^{-1} \right], \quad (11)$$

$$v_0 = \frac{E(2^3S_1) - E(2^3P_0)}{h} = f_{\text{RYD}} \left[\frac{5}{48} \alpha^2 + \frac{\alpha^3}{\pi} \left(\frac{13}{90} + \frac{1}{48} \ln 2 + \frac{3}{16} \ln \alpha^{-1} - \frac{1}{6} \ln R(2,0) + \frac{1}{6} \ln R(2,1) \right) + \frac{1}{48} \alpha^4 \ln \alpha^{-1} \right]. \quad (12)$$

The expressions $\ln R(n,l)$ are the Bethe logarithms [28–30]. Specifically, $\ln R(1,0) = 2.984 128 5$, $\ln R(2,0) = 2.811 769 9$, and $\ln R(2,1) = -0.030 016 7$.

Table I lists the numerical values of the individual terms of the frequencies given in Eqs. (4)–(8), along with the sum of these terms through order $\alpha^3 f_{\text{RYD}}$ and $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$. Table II is a similar listing for the frequency differences. The entries in this table can then be compared to the experimentally measured values presented in Table III. To compute the theoretical numbers the following values [4,5] of the constants appearing in formulas (4)–(12) were used:

$$\alpha^{-1} = 137.035 989 5(61),$$

$$R_\infty = 10973 731.5709(18) \text{ m}^{-1},$$

$$c = 299 792 458 \text{ m/sec},$$

$$f_{\text{RYD}} = cR_\infty = 3 289 841 961.1(5) \text{ MHz}.$$

The present experimentally determined values of v_0 , v_1 , and v_2 test the theory to several parts in 10^4 [31,32]. Since the $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$ coefficient is 1 part in 10^4 for v_2 and several parts in 10^5 for v_0 and v_1 more experimental precision is needed before comparison of the experimental and theoretical values can be used to provide a more stringent test of QED.

Theory and experiment [33] for the $1S$ - $2S$ transitions agree to order $\alpha^3 f_{\text{RYD}}$. To test the $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$ coefficient a more accurate experiment is needed. As previously mentioned, one is being planned with an expected factor-of-10 improvement in accuracy [21]. This new experimental determination of v_{21} will probe the $\alpha^4 \ln \alpha^{-1}$ coefficient.

We should also estimate the order of magnitude of the yet to be calculated $\alpha^4 f_{\text{RYD}}$ term. If we assume that the coefficient scales as $1/n^3$, as it approximately does for the $\alpha^3 f_{\text{RYD}}$ term, we get a contribution to v_{21} of the order of

TABLE II. Numerical values in megahertz of the individual terms in Eqs. (9)–(12). The last two columns are the sums of the terms to order $\alpha^3 f_{\text{RYD}}$ and $\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$.

	f_{RYD}	$\alpha^2 f_{\text{RYD}}$	$\alpha^3 f_{\text{RYD}}$	$\alpha^4 \ln \alpha^{-1} f_{\text{RYD}}$	Total($\alpha^3 f_{\text{RYD}}$)	Total
v_{21}	1 233 690 735.41	-8 2005.59	-1 501.44	-6.69	1 233 607 228.39	1 233 607 221.69
v_2	0.00	8 394.45	230.80	0.96	8 625.25	8 626.21
v_1	0.00	12 774.17	236.74	0.96	13 010.90	13 011.86
v_0	0.00	18 248.81	247.33	0.96	18 496.14	18 497.10

TABLE III. Experimental values in megahertz of the frequency differences corresponding to Eqs. (9)–(12).

Frequency difference	Brandeis [30]	Michigan [31]	Bell Labs [32]
ν_{21}			1 233 607 218.9(10.9)
ν_2	8 628.4(2.8)	8 619.6(2.7)(0.9)	
ν_1		13 001.3(3.9)(0.9)	
ν_0		18 504.1(10.0)(1.7)	

$\frac{7}{8}(\alpha^4/\pi)f_{\text{RYD}} \sim 2.60$ MHz. This is 2.1 ppb (parts per 10^9) which is in the range of the accuracy of the new experiment. Consequently, the complete $(\alpha^4/\pi)f_{\text{RYD}}$ term must be calculated, a task which the author is currently pursuing.

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