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Complete Results for Positronium Energy Levels at Order $m\,\alpha^6$

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Abstract

We have completed theoretical predictions for positronium energy levels through order $m\,\alpha^6$ by the calculation of the spin independent radiative recoil correction. This contribution is significant and amounts to 10.64 MHz for the 1S state. We further perform a detailed comparison of theoretical predictions to experimental results for $1S-2S$ and $2S-2P$ transitions. There is a serious discrepancy between previous theoretical results for the hfs of the ground state and with corresponding experiments. This problem remains to be resolved.

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Positronium is an unique hydrogenic atom with which to study quantum electrodynamic (QED) effects in bound systems. The small mass of the electron ensures that strong and weak interaction effects contribute at a negligible level. The energy spectrum may therefore be predicted with an accuracy limited only by the complexity in the higher order QED calculations. The equal mass of the electron and the positron requires a special theoretical treatment to incorporate relativistic and recoil effects on the same footing. Moreover, the existence of annihilation channels also affects the energy levels. Therefore, the calculation of higher order corrections presents a challenge to the development of quantum electrodynamics. Recently significant progress has been achieved through the complete calculation of single photon annihilation contribution to positronium hyperfine splitting (*hfs*) by Adkins *et al.* [1] and Hoang *et al.* [2], and a pure recoil contribution [3] to S-level energies. In this letter we report the calculation of the last unknown correction to positronium S-levels in order $m\,\alpha^6$, the spin independent radiative recoil contribution. Having evaluated it, we give theoretical predictions in Table I for six transitions in positronium which are experimentally known with high accuracy. In the conclusion we emphasize that although current predictions are now more accurate than experimental values, there are discrepancies between different theoretical calculations that have yet to be resolved.

The radiative recoil corrections are in general difficult to treat. A rigorous derivation starts from the Bethe-Salpeter equation, and incorporates radiative corrections in the kernel [15]. In order $m\,\alpha\,(Z\,\alpha)^5$ a simplified treatment is sufficient. One finds an effective interaction potential between the electron and the positron from the corresponding S-matrix amplitude. When this amplitude is infrared divergent, then a separate treatment is necessary for small photon momenta. An illustrative example is the one–loop contribution to the hydrogen Lamb shift of order $m\,\alpha\,(Z\,\alpha)^4$, where the low energy part leads to the well known Bethe logarithm. In a higher order $m\,\alpha\,(Z\,\alpha)^5$ this low energy part is simply absent. In the case of positronium we calculate the forward two-photon exchange electron-positron scattering amplitude at zero spatial components of the momenta. Nonperturbative effects enter only in lower order. This simplified treatment has been justified in Ref. [16]. Similar calculations have also been performed for positronium *hfs* in Ref. [17], and for radiative recoil corrections to the Lamb shift in hydrogen in Ref. [18].

We start the calculation by considering the vacuum polarization effect. It modifies one of the photon propagators, which gives a small energy shift. Our result is [19]:

$$\Delta E(nS) = \frac{m\,\alpha^6}{n^3}\left(\frac{1}{36} - \frac{5}{27\,\pi^2}\right)\,, \tag{1}$$

in agreement with the former result in Ref. [20]. The electron and the positron self–energy corrections to positronium S–levels can be written in the form [21]

$$\Delta E(nS) = -\frac{m^3\,\alpha^6}{\pi\,n^3}\int\frac{d^4q}{\pi^2\,i}\,\mathcal{L}(q)\,, \tag{2}$$

$$\mathcal{L}(q) = \frac{q^2\,T_0^0(q) + q_0^2\,T_\mu^\mu(q)}{q^4\,(q^4 - 4\,m^2\,q_0^2)}\,, \tag{3}$$

where T^μ_ν is a radiatively corrected (off–shell) Compton amplitude, which was calculated analytically in Ref. [18]. The integration is done along the Feynman contour. The expression in Eq. (3) requires subtraction of terms that were included in the leading order self–energy contribution of order $m\,\alpha^5$,

$$\mathcal{L} \approx \frac{-\frac{10}{9} + \frac{4}{3}\ln\left[(\boldsymbol{q}^2 - 2\,m\,q_0)/m^2\right]}{\pi\,(\boldsymbol{q}^2 - 2\,m\,q_0)^2\,(\boldsymbol{q}^2 + 2\,m\,q_0)}\,. \tag{4}$$

The integral in Eq. (2) with the subtracted $\mathcal{L}$ is finite and amounts to

$$\Delta E(nS) = \frac{m\,\alpha^6}{\pi^2\,n^3}\left[-\frac{35}{16} + \frac{31}{48}\,\pi^2 + \frac{9}{8}\,\zeta(3)\right]\,. \tag{5}$$

All other corrections up to the order $m\,\alpha^6$ have already been calculated, so we can now present improved theoretical predictions.

The main structure of the positronium spectrum is obtained from the nonrelativistic Hamiltonian. The leading relativistic effects of order $m\,\alpha^4$ are known for arbitrary positronium states [22]. Corrections of order $m\,\alpha^5$, including Lamb shift-like effects, recoil, and annihilation contributions were calculated in Refs. [23,24]. A useful summary of these results can be found in Ref. [25]. Recently Khriplovich and coworkers have calculated all $m\,\alpha^6$ corrections to P-levels in Ref. [26], using the Breit formalism. In the case of S-states the calculation is much more complex. The logarithmic terms $m\,\alpha^6\,\ln(\alpha)$ come from the single photon annihilation channel [27] and from the spin dependent part of photon exchange contributions [28]. The spin independent part, as was found in Refs. [25,29], does not lead to $\ln(\alpha)$ terms. Values for nonlogarithmic corrections are displayed in Table II. We divide them into 1–, 2–, 3– photon annihilation terms, and 0–, 1–, 2– radiative loop exchange terms. Additionally, photon exchange terms have spin independent and spin dependent parts, proportional to the operator $\boldsymbol{s}_-\boldsymbol{s}_+$, that lead to the hyperfine splitting.

The photon annihilation terms have been calculated for the *hfs*. The contribution to energy levels from these terms can be found by noting that 1– and 3–photon annihilation diagrams contribute only to orthopositronium and 2–photon to parapositronium, as shown in Table II. One-photon annihilation diagrams have been investigated in detail in Refs. [30–32] and the calculation has recently been completed. Most of the annihilation terms are state independent, *i.e.* they behave as $1/n^3$. The one–photon annihilation brings in a nontrivial state dependence. The complete formula, as derived by Hoang *et al.* in Ref. [2] is

$$\begin{aligned}\Delta E(n^3S_1) = \frac{m\,\alpha^6}{n^3}\biggl\{&\frac{1}{24}\ln(\alpha^{-1})\; - 0.1256487\\ &+\frac{1}{24}\left[\ln(n) - \Psi(n) + \Psi(1)\right]\\ &+\frac{1-n}{24\,n} - \frac{37}{96}\,\frac{1-n^2}{n^2}\biggr\}\,,\end{aligned} \tag{6}$$

where $\Psi(n)$ is the logarithmic derivative of the Euler Γ-function. The value for $n = 1$ has been independently calculated by Adkins *et al.* [1], which provides a crucial check for this complicated calculation. Since the state dependent part is surprisingly large we recalculated it and got agreement with Eq. (6). The state dependence of the vacuum polarization contribution was also calculated in Ref. [33]. Two-photon and three-photon annihilation contributions are state independent and the final results after correcting previous calculations are presented in Refs. [34] and [35] respectively.

The photon exchange contributions to the hyperfine structure are presented as a spin dependent part in Table II. The two–loop radiative term is given by the α^2 part of $(1+a_e)^2$, where a_e is the electron anomalous magnetic moment. Single radiative loop exchange, *i.e.* the radiative recoil correction $(m\,\alpha\,(Z\alpha)^5)$ was obtained numerically in Ref. [17]. We have recalculated it analytically, and obtained a result

$$\Delta E(nS) = \frac{m\,\alpha^6}{\pi^2\,n^3}\,\boldsymbol{s}_-\boldsymbol{s}_+\left[\frac{41}{36}-\frac{79}{48}\,\pi^2+\frac{4}{3}\,\pi^2\,\ln(2)+\frac{\zeta(3)}{2}\right]. \tag{7}$$

The numerical value -0.54535 slightly differs from the former result in Ref. [17], -0.5394(14). The pure recoil contribution $((Z\alpha)^6\,m)$, which is state dependent, was evaluated in Ref. [13] for $n=1$, but has been recently recalculated for all nS states in Ref. [14]

$$\begin{aligned}\Delta E(nS) = \frac{m\,\alpha^6}{n^3}\,\boldsymbol{s}_-\boldsymbol{s}_+ \Biggl\{&\frac{1}{6}\,\ln(\alpha^{-1})\;+0.3767(17)\\ &+\frac{1}{6}\bigl[\ln(n)-\Psi(n)+\Psi(1)\bigr]\\ &+\frac{7}{12}\,\frac{1-n}{n}-\frac{1-n^2}{2\,n^2}\Biggr\},\end{aligned} \tag{8}$$

where

$$\boldsymbol{s}_-\boldsymbol{s}_+ = \begin{cases}\;\;1/4 \text{ for triplet,}\\ -3/4 \text{ for singlet.}\end{cases} \tag{9}$$

These two results [0.167(33) versus 0.3767(17)] are in serious disagreement at $n=1$. In Table II and below, we include results of Ref. [14], but in Table I both contradicting results are presented for the ground state *hfs*.

The spin independent part of the photon exchange contributions can be also classified as $m\,\alpha^2(Z\alpha)^4$, $m\,\alpha(Z\alpha)^5$ and $m\,(Z\alpha)^6$ terms. The first one, a single photon exchange, can be found from the well-known two-loop expression for the hydrogen Lamb shift, taking into account the reduced mass effect and multiplying the self-energy by a factor 2. The radiative recoil contribution, $m\,\alpha(Z\alpha)^5$, is calculated in this work. It is the sum of Eqs. (5) and (1), and is included in Table II. As was also the case for *hfs* [17], the self energy contribution is relatively large compared to all other terms. The last term, $(m\,(Z\alpha)^6)$, the pure recoil contribution, has been recently calculated in Ref. [3]. This correction is state dependent and amounts to

$$\begin{aligned}\Delta E(nS) = \frac{m\,\alpha^6}{n^3}\Biggl\{&-0.31056(63)\\ &-\frac{1-n}{4\,n}+\frac{1-n^2}{3\,n^2}-\frac{69}{512}\,\frac{1-n^3}{n^3}\Biggr\}.\end{aligned} \tag{10}$$

The sum of all constant $m\,\alpha^6$ terms for 1S and 2S states is (see Table II)

$$E^{(6)}(1S) = m\,\alpha^6\left[0.16107(63)-0.3925(17)\,\boldsymbol{s}_-\boldsymbol{s}_+\right], \tag{11}$$

$$E^{(6)}(2S) = \frac{m\,\alpha^6}{8}\left[0.34557(63)-0.1048(17)\,\boldsymbol{s}_-\boldsymbol{s}_+\right]. \tag{12}$$

The significant state dependence comes mainly from the 1–photon annihilation contribution. As an example, the $m\,\alpha^6$ term contributes 0.75 MHz for 2^3S_1 state.

Unknown higher order terms limit the precision of theoretical predictions. The double logarithmic term $m\,\alpha^7\,\ln^2(\alpha)$ is known only for the hyperfine structure and annihilation contributions [39], and is included in the theoretical value for the *hfs* in Table I. In the case of the spin independent part the double logarithmic contribution is unknown. We estimate it as 1 MHz for the ground state by scaling the well known non-recoil correction to the hydrogen Lamb shift with the reduced mass factor $(\mu/m)^3$. As an example current theoretical predictions for the $1S-2S$ transition is:

$$E(2^3S_1) - E(1^3S_1) = 1233\,607\,221.0(1.0)\ \text{MHz}\,, \tag{13}$$

where we use $\alpha^{-1} = 137.035\,999\,93(52)$ [40] and $c\,R_\infty = 3\,289\,841\,960.394(27)$ MHz [41]. This result is in moderate agreement with the experiment [5]

$$E(2^3S_1) - E(1^3S_1) = 1233\,607\,216.4(3.2)\ \text{MHz}\,. \tag{14}$$

The corrections of order $m\,\alpha(Z\alpha)^5$ (Eqs. (1) and (5)) contribute a significant amount, -9.31 MHz, to this transition. The comparison of theoretical predictions to a less precise $1S-2S$ measurement [4] as well as for the $2S-2P$ experiments is presented in Table I. In all cases theoretical predictions are more precise. The $2S-2P$ transitions are weakly affected by the discrepancy in theoretical predictions, *i.e.* by about 0.01 MHz. Experimental results of Refs. [9–11] are in agreement with theoretical predictions, while the results of Ref. [8] are in slight disagreement. The hyperfine structure measurements are in agreement with the Caswell and Lepage result [27] and in 3.4 standard deviation disagreement with Ref. [14]. This disagreement could not be resolved by comparison of the $1S-2S$ transition, since it is not sufficiently sensitive to *hfs* contributions, see Eq. (9).

The evaluation of the $m\,(Z\alpha)^6$ contribution was a complicated task. Both calculations of positronium *hfs* at this order, Refs. [27] and [14], reproduce in the limit of heavy nucleus mass M known results both in the orders of $(Z\alpha)^6 m^2/M$ and $(Z\alpha)^6 m^3/M^2$ [36]. Moreover, the result of Ref. [14] is in agreement with the state dependent terms of these orders calculated in Refs. [37] and [38] respectively. The discrepancy between these works will have to be resolved before final conclusions can be drawn.

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TABLES

Transition	Exp. Refs.	Experiment [MHz]	Theory [MHz]	Difference [MHz]
$2^3S_1 - 1^3S_1$	[4]	1233 607 218.9 (10.7)	1233 607 221.0 (1.0)	2.1(10.7)(1.0)
	[5]	1233 607 216.4 (3.2)		4.6(3.2)(1.0)
$1^3S_1 - 1^1S_0$	[6]	203 387.5 (1.6)	203 388.09 (0.80) ^{a}	0.6(1.6)(0.8) ^{a}
			203 392.02 (0.50) ^{b}	4.5(1.6)(0.5) ^{b}
	[7]	203 389.10 (0.74)		-1.01(0.74)(0.80) ^{a}
				2.92(0.74)(0.50) ^{b}
$2^3S_1 - 2^3P_0$	[8]	18504.1 (10.0)(1.7)	18498.42(0.13)	-5.7(10.0)(1.7)
	[9,10]	18499.65 (1.20)(4.00)		-1.2(1.2)(4.0)
$2^3S_1 - 2^3P_1$	[8]	13001.3 (3.9)(0.9)	13012.58(0.13)	11.3(3.9)(0.9)
	[9,10]	13012.42(0.67)(1.54)		0.2(0.7)(1.5)
$2^3S_1 - 2^3P_2$	[8]	8619.6(2.7)(0.9)	8626.87(0.13)	7.3(2.7)(0.9)
	[11]	8628.4(2.8)		-1.5(2.8)
	[9,10]	8624.38(0.54)(1.40)		2.5(0.5)(1.4)
$2^3S_1 - 2^1P_1$	[12]	11181(13)	11185.54(0.13)	5(13)
	[10]	11180(5)(4)		6(5)(4)
$2^3S_1 - 2^1S_0$	not measured yet		25424.69(0.06) ^{b}	

TABLE I. Comparison of experiments to theoretical predictions. In case of the fine structure we give statistical and systematic errors separately because some data in Table are correlated. Theoretical results for the ground state *hfs* were given in Refs. [1] and [2]. References to contradicting theoretical works are: ^{a} – [13]; ^{b} – [14]. Theoretical uncertainties are dominated by estimates for unknown higher order terms. The differences for $2S - 2P$ are presented without theoretical uncertainties, since they are significantly smaller than experimental ones. The levels are labeled as $n^{2S+1}L_J$.

Contribution	K	$\Delta E(1^1S_0)$ [MHz]	$\Delta E(1^3S_1)$ [MHz]
$1\,\gamma$	$-0.12565\,\left(\frac{3}{4}+\boldsymbol{s}_-\boldsymbol{s}_+\right)$	0	-2.34
$2\,\gamma$	$0.03248\,\left(\frac{1}{4}-\boldsymbol{s}_-\boldsymbol{s}_+\right)$	0.61	0
$3\,\gamma$	$-0.05194\,\left(\frac{3}{4}+\boldsymbol{s}_-\boldsymbol{s}_+\right)$	0	-0.97
$\alpha^2\,(Z\alpha)^4\,m$	$0.02647-0.01374\,\boldsymbol{s}_-\boldsymbol{s}_+$	0.69	0.43
$\alpha(Z\alpha)^5\,m$	$0.57023-0.54535\,\boldsymbol{s}_-\boldsymbol{s}_+$	18.27	8.10
$(Z\alpha)^6\,m$	$-0.31056(63)+0.3767(17)\,\boldsymbol{s}_-\boldsymbol{s}_+$	-11.07(2)	-4.04(1)
total	$0.16107(63)-0.3925(17)\,\boldsymbol{s}_-\boldsymbol{s}_+$	8.50(2)	1.17(1)

TABLE II. All constant $m\,\alpha^6$ contributions to the $1S$ state. The spin dependent part is similar to that in Ref. [1], although we use a different naming. Results are presented both in relative units of $K\,m\,\alpha^6$ and in frequency units.