Corrections to the measured $n = 1$ hyperfine interval of positronium due to annihilation effects

A. Rich
*Physics Department, University of Michigan, Ann Arbor, Michigan 48109**
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The existence of corrections, due to annihilation, to the usual expressions for the energy levels and decay rates of the $m = 0$ triplet and singlet states of positronium in a magnetic field are noted. The corrections cause the value of the hyperfine interval ν, as obtained from well-known resonance experiments, to increase by 1.8 standard deviations of the current experimental error to $\nu = 203\,387.5(1)$ MHz where $\nu(\text{theor}) = 203\,400(10)$ MHz. This shift could be observable in the near future when calculations of ν to order α^2 are completed.

The weighted mean value of the three most recent measurements[1-3] of the $n = 1$ hyperfine interval of positronium is $\nu = 203\,385.7(1)$ MHz (5 ppm). The error quoted is the weighted mean error obtained from the quoted standard deviations. An experiment to improve this accuracy to 3 ppm is now nearing completion.[4] The comparison of the above experimental value with the theoretical calculation is important as a test of quantum electrodynamics in a purely leptonic, self-annihilating, bound system. The comparison also tests the Bethe-Salpeter equation and more recent formulations of the relativistic two-body problem[5-8] in a system where reduced mass and recoil effects are at a maximum and where the only interaction present at the levels of accuracy of interest is that of electrodynamics.

The theoretical determination of the hyperfine interval ν has been completed through the order α and $\alpha^2 \ln\alpha^{-1}$ radiative corrections with a number of classes of diagrams of order α^2 also calculated.[5-7,9] The result for ν including all diagrams of order α and $\alpha^2 \ln\alpha^{-1}$ is

$$\nu = (\alpha^2 cR)\left[\frac{7}{6} - \frac{\alpha}{\pi}\left(\frac{16}{9} + \ln 2\right) + \frac{5}{12}\alpha^2 \ln\alpha^{-1} + \cdots\right]$$
$$= 203\,400.4 \qquad (1)$$

expressed in units of MHz (0.22 ppm). The values of α, R, and c used to obtain the above numerical result have errors of 110, 3, and 4 ppb (parts per billion), respectively.[10] The error for ν quoted is simply due to the errors in these constants. Of much greater importance is the fact that the order α^2 radiative corrections are only partially calculated so that the current theoretical uncertainty in ν must be taken as of order α^2 (50 ppm or 10 MHz). We note, however, that a very vigorous attack on a complete calculation of the order α^2 terms is now in progress and it is entirely possible that ν will be known to about 1 ppm (the magnitude of the next-higher-order diagrams, $\alpha^3 \ln^2\alpha^{-1}$, is of order 10^{-6}) in the near future.[11]

In view of the forthcoming possibility of a comparison of experiment and theory at the few-ppm level, it is important to consider any corrections to the current experimental analysis at this level. Such a correction is the effect of the decay of Ps on the central value of the resonance and on the resonance line shape observed in the experiments. This effect, implicit, though not discussed, in an early calculation[12] related to Ps decay in magnetic fields, was mentioned qualitatively in one of the initial articles[13] reporting a measurement of ν, and is discussed briefly in a recent paper.[14] The purpose of this article is to present exact expressions, corrected for decay, for the energy levels and perturbed lifetimes of ground-state Ps in a magnetic field. The major result of these calculations is that the magnitude of the shift in the triplet energy level is sufficiently large (9 ppm) so that it must be included in the current analysis of the hyperfine separation. A shift of similar size also occurs in the singlet energy level and in the triplet ($m = 0$) decay rate while a smaller shift occurs in the singlet decay rate. These shifts are unobservable at the present levels of experimental accuracy. Finally, we point out that the results of a recent numerical evaluation of the rf line shape, including decay, suggest the need for a line shape recalculation to the ppm level of accuracy.

In order to compare the new expressions with those used previously and to establish notation we first write down the previous solutions for Ps in an external magnetic field. The spin-wave functions of $n = 1$ Ps in zero field may be represented in the singlet, triplet representation as $\psi_S = 2^{1/2}(\uparrow\ddagger - \downarrow\dagger)$, $\psi_T(m=1) = \uparrow\dagger$, $\psi_T(m=-1) = \downarrow\ddagger$, and $\psi_T(m=0) = \psi_T(0) = (2^{-1/2})(\uparrow\ddagger + \downarrow\dagger)$ where $\uparrow, \dagger$ refer to electron, positron spin, respectively, and m denotes the projection of spin onto an arbitrary quantization axis. These states are split into energy levels W_T and W_S (W_S is taken as the zero of energy in what follows) which are separated by the quantity of interest ν, i.e., $W_T = W = h\nu$. The singlet state decays primarily into two antiparallel γ quanta with a calculated decay rate $\lambda_S = 7.98 \times 10^9\ \text{sec}^{-1}$ while the triplet states decay primarily into three γ's at the calculated rate $\lambda_T = 7.04 \times 10^6$ sec^{-1}. In the presence of a static magnetic field B oriented along the z axis the magnetic part of the Hamiltonian is given by $H_M = \frac{1}{2} g' \mu_B B[\sigma_z(e^-) - \sigma_z(e^+)]$. Here μ_B is the Bohr magneton, $\sigma_z(e^-)$ and $\sigma_z(e^+)$ the Pauli-spin matrices for electron and position, and account is taken of quantum electrodynamic effects (the g-factor anomaly a) as well as relativistic binding and center-of-mass motion effects[15] by writing $\frac{1}{2} g' = (1+a)\,[1 - \frac{5}{24}\alpha^2 - T(\mathrm{c.m.})/2mc^2]$. Symmetry considerations[16] show that the magnetic field has no effect on the $\psi_T(\pm 1)$ states, but does mix $\psi_T(0)$ and ψ_S to give perturbed eigenstates ψ_T' and ψ_S' with corresponding energies W_T' and W_S' and decay rates λ_T' and λ_S'. Diagonalization of the energy matrix including H_M, but neglecting decay, lead to Breit-Rabi-type expressions for the field-perturbed eigenstates and energies. The perturbed decay rates are then written down by considering for (λ_T', λ_S') the fraction of (ψ_S, ψ_T) mixed into (ψ_T', ψ_S'). The results are[12,13,17]

$$\psi_T' = (1+y^2)^{-1/2}[\psi_T(0) + y\psi_S] \ , \tag{2a}$$

$$\psi_S' = (1+y^2)^{-1/2}[\psi_S - y\psi_T(0)] \ , \tag{2b}$$

$$W_T' = \frac{1}{2} W_T[1 + (1+x^2)^{1/2}] \underset{x \ll 1}{\simeq} W(1 + \tfrac{1}{4}x^2) \ , \tag{2c}$$

$$W_S' = \frac{1}{2} W_T[1 - (1+x^2)^{1/2}] \underset{x \ll 1}{\simeq} -\tfrac{1}{4}x^2 W \ , \tag{2d}$$

$$\lambda_T' = \frac{1}{1+y^2}(\lambda_T + y^2\lambda_S) \ , \tag{2e}$$

$$\lambda_S' = \frac{1}{1+y^2}(\lambda_S + y^2\lambda_T) \ . \tag{2f}$$

Here $x = 2g'\mu_B B/W \simeq B/36.5$ kG and $y = x/[1 + (1+x^2)^{1/2}]$.

The technique used to measure ν consists of forming Ps in a static magnetic field B (typically $B \sim 8$–10 kG) and then applying an rf magnetic field $B_y \cos(2\pi f t)$ perpendicular to B. For technical convenience B (i.e., x) rather than f is then varied and when for a fixed f $(f = f_0)$, $W_T'(x)$ satisfies the approximate condition

$$W_T' - W = hf_0 = \tfrac{1}{2} h\nu[(1+x^2)^{1/2} - 1] \tag{3}$$

transitions $\psi_T(\pm 1) \rightleftarrows \psi_T'$ are induced. Since $\lambda_T' \sim 15\lambda_T$ at $B \sim 8$ kG, the transition $\psi_T(\pm 1) \rightarrow \psi_T'$ predominates if B_y is chosen so that the transition rate (λ_{rf}) for the process is much less than λ_T', but of order λ_T [typically $B_y \sim 10$ G implying $\lambda_{\mathrm{rf}} \sim \frac{1}{2}\lambda_T \sim (2-3)\times 10^{-2}\lambda_T'$]. The $\psi_T(\pm 1) \rightarrow \psi_T'$ transition causes an increase (decrease) in the $2\gamma(3\gamma)$ decay fraction since at the value of B used ψ_T' decays primarily into 2 γ's. Detection of the change in one or the other of these fractions with B yields an approximately Lorentzian resonance line whose fractional natural linewidth under the conditions obtaining in the experiment $(x \sim \frac{1}{4},\ x^2\lambda_S >> \lambda_T)$ may be written as

$$\delta B/B = (\lambda_T' + \lambda_T)/4\pi f_0 \simeq \lambda_S/4\pi\nu = 3.1 \times 10^{-3} \ .$$

Using Eq. (3) one determines ν from the measured value of f_0 and the value of B (i.e., x) as obtained from the peak in the fitted resonance curve. Corrections to Eq. (3) due to the fact that ψ_T and ψ_T' represent decaying states are therefore reflected in the value of ν obtained from the measured f_0. These corrections as well as corrections to W_S', λ_T', and λ_S' will now be discussed.

The most direct procedure for obtaining the complex energy eigenvalues of Ps in a magnetic field is to diagonalize the magnetic submatrix including decay, which written in the ψ_S, $\psi_T(0)$ basis is

$$H_M(d) = \begin{pmatrix} \mathcal{W}_S & \dfrac{xW}{2} \\ \dfrac{xW}{2} & \mathcal{W}_T \end{pmatrix} \ . \tag{4}$$

Here $\mathcal{W}_S = -i\hbar\lambda_S/2$, $\mathcal{W}_T = W - i\hbar\lambda_T/2$, and the off-diagonal elements of $H_M(d)$ are $\langle\psi_S|H_M|\psi_T(0)\rangle = \langle\psi_T(0)|H_M|\psi_S\rangle = xW/2$. The (complex) eigenvalues of $H_M(d)$ associated with ψ_S' and ψ_T' are

$$\mathcal{W}_{T,S}' = \tfrac{1}{2}[(\mathcal{W}_T + \mathcal{W}_S) \pm (\mathcal{W}_T - \mathcal{W}_S)(1+z^2)^{1/2}] \ . \tag{5}$$

Here the $(+,-)$ refer to $(\mathcal{W}_T', \mathcal{W}_S')$ and $z = x(1-ig)/(1+g^2)$, $g = (\lambda_S - \lambda_T)/4\pi\nu = 3.1 \times 10^{-3}$.

The energy eigenvalues and decay rates of ψ_T' and ψ_S' obtained from $\mathcal{W}_T'$ and $\mathcal{W}_S'$ are given by $(\hbar = 1)$

$$W_T'(d) = \mathrm{Re}\mathcal{W}_T' = \tfrac{1}{2}(W + C) \ , \tag{6a}$$

$$W_S'(d) = \mathrm{Re}\mathcal{W}_S' = \tfrac{1}{2}(W - C) \ , \tag{6b}$$

$$\lambda_T'(d) = -2\,\mathrm{Im}\mathcal{W}_T' = (\lambda_S + \lambda_T) - 2D \ , \tag{6c}$$

$$\lambda_S'(d) = -2\,\mathrm{Im}\mathcal{W}_S' = (\lambda_S + \lambda_T) + 2D \ . \tag{6d}$$

Here $C = \{[a + (a^2+b^2)^{1/2}]/2\}^{1/2}$ and $D = \{[-a + (a^2+b^2)^{1/2}]/2\}^{1/2}$ with $a = W^2[(1-g^2) + x^2]$ and $b = 2gW^2$. Clearly z is the complex analog of x and the effect of decay is seen to change the magnitude of z by order $g^2 \simeq 9$ ppm. The size of g^2 immediately sets the scale of the perturbation caused by decay, however, in order to explore the effect quantitatively, it is useful to expand through order g^2. The result, valid for all x is

$$f_0(d)=\frac{W_T'(d)-W}{2\pi}$$
$$=\tfrac{1}{2}\nu\left\{\left[1-\frac{1}{2}\left(\frac{xg}{1+x^2}\right)^2+O(g^4)\right](1+x^2)^{1/2}-1\right\}\ , \tag{7a}$$

$$\lambda_T'(d)=\lambda_T'-\gamma$$
$$=\lambda_T'-\frac{1}{4}\left(\frac{(\lambda_S-\lambda_T)}{(1+x^2)^{1/2}}\right)\left[\left(\frac{xg}{1+x^2}\right)^2+O(g^4)\right]\ , \tag{7b}$$

$$W_S'(d)=\tfrac{1}{2}W\left\{1-(1+x^2)^{1/2}\left[1-\frac{1}{2}\left(\frac{xg}{1+x^2}\right)^2+O(g^4)\right]\right\}\ , \tag{7c}$$

$$\lambda_S'(d)=\lambda_S'+\gamma\ . \tag{7d}$$

We see [Eq. (7a)] that through $O(g^2)$ the fractional effect of decay on f_0 is given by

$$\frac{f_0-f_0(d)}{f_0}=\frac{1}{2}\left(\frac{xg}{1+x^2}\right)^2\left(\frac{(1+x^2)^{1/2}}{(1+x^2)^{1/2}-1}\right)$$
$$\underset{x\ll 1}{\simeq} g^2[1-\tfrac{3}{2}x^2+O(x^4)]\ ,$$

i.e., decay decreases the energy separation between ψ_T and ψ_T' by approximately $g^2=9.7$ ppm in the limit of $x \ll 1$. Consequently the value of ν obtained from this splitting should be increased in the same proportion, *if inclusion of decay in H_M does not also cause a change in the line shape for the rf resonance situation.* The values of x which characterize the two most recent determinations of f_0 are $x=0.25$ (Ref. 1) and $x=0.22$.[2,3] The values of ν obtained from the measured values of $f_0(d)$ and Eq. (7a) are accordingly from Ref. 1, $\nu(1)=203\,388.7(1.6)$ MHz and from Ref. 2, $\nu(2)=203\,386.7(1.2)$ MHz, i.e., $\nu(1)$ and $\nu(2)$ must be adjusted upwards by approximately 9 ppm (1.7 and 1.8 MHz, respectively). A new average value for the hyperfine interval may therefore be given as $\nu=203\,387.5(1)$ MHz. This change from the current value of $\nu=203\,385.7(1)$ MHz may be observable when the α^2 terms in the theoretical expression for ν [Eq. (1)] are calculated.

Finally we note that, as can be readily determined from Eqs. (7b)–(7d), the fractional changes in W_S', λ_T', and λ_S' due to the inclusion of annihilation in H_M are, for the conditions which obtain in the hfs experiments ($x\sim\frac{1}{4}$), $[W_S'(d)-W_S']/W_S'\simeq -g^2$, $[\lambda_T'(d)-\lambda_T']/\lambda_T'\simeq -0.9g^2$, and $[\lambda_S'(d)-\lambda_S']/\lambda_S'\simeq +(xg/2)^2$. Deviations of this order would be unobservable in either the hfs experiment or in direct measurements of λ_T' which are currently being performed at Michigan and Mainz.[14] The value of the only one of these ratios which might be susceptible to a precision measurement $[\lambda_T'(d)-\lambda_T']/\lambda_T'$, is in fact less than g^2 for all x. Consequently, the deviation of this ratio from zero will probably be unobservable in the foreseeable future.

Note added. It was pointed out to the author[18] that a numerical calculation of the line shape discussed in the text may be found in the literature.[19] The effect of decay on the resonance peak was not discussed in Ref. 19, but Dr. Mills informs me that the calculation has been carried out with the result that to 0.5 ppm there is *no shift* of the frequency from the value of f_0 given by Eq. (3). This is a most interesting result of possibly general interest. When coupled with the calculation of this article, it suggests that a review of the line-shape theory is necessary.

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*Present address: Institut des Hautes Études Scientifiques, 91440 Bures-sur-Yvette, France.

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