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CORRECTIONS TO THE POSITRONIUM HYPERFINE STRUCTURE OF ORDER $\alpha^2 \ln\alpha^{-1}$ †

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We report a calculation of the $m\alpha^6 \ln\alpha^{-1}$ contributions to the triplet-singlet splitting of the positronium ground state. Our result,

$$\Delta\nu(\alpha^6 \ln\alpha^{-1}) = \tfrac{1}{2} m\alpha^6 \ln\alpha^{-1} = 46 \text{ MHz},$$

shifts the theoretical prediction from two standard deviations below to two standard deviations above the most recent experimental value.

We would like to give a preliminary report of a calculation of the $m\alpha^6 \ln\alpha^{-1}$ contributions to the ground-state triplet-singlet splitting of positronium (the positronium "hyperfine structure"). Our result for the frequency contribution $\Delta\nu$ in this order is

$$\Delta\nu = \tfrac{1}{2} m\alpha^6 \ln\alpha^{-1}, \tag{1}$$

where $\hbar = c = 1$. Including this contribution, the total triplet-singlet transition frequency becomes

$$\nu = \alpha^2 \mathrm{Ry}_\infty \left[\frac{7}{6} - \left(\frac{16}{9} + \ln 2\right)\frac{\alpha}{\pi} + \alpha^2 \ln\alpha^{-1} + O(\alpha^2)\right]. \tag{2}$$

The energy levels of the ground state of positronium have been calculated by a number of authors.[1-3] Karplus and Klein[3] were the first to evaluate completely all corrections of order $m\alpha^5$ to the triplet-singlet splitting. Their results agreed with the experimental data available at the time,[4-6] but disagree with the more precise data which were recently obtained.[7] This discrepancy between experiment and theory motivated our higher order calculation.

The positronium results to order $m\alpha^4$ present no difficulties and can be considered well established. We believe that the same can be asserted for the $m\alpha^5$ calculations of Karplus and Klein, although we have not rechecked these results in detail. In this connection, we would like to call attention to the Fulton and Martin[8,9] calculation of electrodynamic corrections to the energy levels of a system of two fermions with arbitrary masses. The results of these authors (with annihilation effects included), when applied to the ground state of positronium, agree with the $m\alpha^5$ terms obtained by Karplus and Klein. Moreover, they also agree with the corresponding hydrogen Lamb shift to this order,[10] with recoil corrections to the Lamb shift,[11,12] and with the calculations by Arnowitt[13] of the hyperfine structure contributions for an arbitrary-mass two-fermion system. Thus, the work of Fulton and Martin intimately ties the $m\alpha^5$ positronium results to a number of by now well-established results for hydrogen (and deuterium) spin, orbit, and spin-orbit effects.

The contributions of order $m\alpha^6 \ln\alpha^{-1}$ represent recoil corrections arising from low-momentum

components of the wave function associated with the Bethe-Salpeter equation[14] for positronium. The perturbation techniques used by Karplus and Klein[3] and by Fulton and Karplus[15] prove sufficiently accurate to this order. The wave function needed is that obtained from the Bethe-Salpeter equation, containing only the Coulomb interaction, and involves a single iteration from the nonrelativistic Pauli wave function. This wave function, which is implicitly stated in earlier work,[3,9,11,15] is explicitly expressed to a higher accuracy in the wave-function momentum than was previously necessary. We must also keep other momentum contributions to a higher order. On the other hand, retardation effects in the wave function can be neglected to our order and wave-function pair effects are also negligible in the two-photon–exchange contributions. However, it is essential that these two effects are taken into account in the interaction kernels.

We have carried out a systematic study of all relevant terms and believe that the only Feynman diagrams which contribute to our order are those involving the exchange of one or two (crossed and uncrossed) virtual transverse photons. Diagrams involving three virtual photons are at least of order $m\alpha^6$. Of course, there are numerous other $m\alpha^6$ contributions due to recoil (and also involving wave-function pair and retardation effects) from lower order diagrams. At first sight, the calculation of all $m\alpha^6$ effects appears to be unmanageably difficult. This is not the case in the order $m\alpha^6\ln\alpha^{-1}$. All expressions encountered can be completely evaluated analytically. The contributions from the various diagrams to the energy separation are found to be

$$\tfrac{1}{8}m\alpha^6\ln\alpha^{-1} \text{ for single-photon exchange,} \quad (3)$$

and

$$\tfrac{3}{8}m\alpha^6\ln\alpha^{-1} \text{ for two-photon exchange.} \quad (4)$$

Table I summarizes the various theoretical contributions to the positronium energy levels in the ground state. The value of the fine-structure constant is taken to be[16]

$$\alpha^{-1} = 137.036\,08. \quad (5)$$

The first line, corresponding to the ionization energy, is not really relevant to the triplet-singlet splitting, and is only included for completeness. Thus, it is not surprising nor disturbing that the largest discrepancy between columns two and three occurs in the second line. Column three is computed using the simple rules

$$\nu_{\rm est}(\alpha^4) = \alpha^2\nu_{\rm calc}(\alpha^2), \quad \nu_{\rm est}(\alpha^5) = \alpha\nu_{\rm calc}(\alpha^4),$$
$$\nu_{\rm est}(\alpha^6\ln\alpha^{-1}) = \alpha\ln\alpha^{-1}\nu_{\rm calc}(\alpha^5), \quad \nu_{\rm est}(\alpha^6) = (\ln\alpha^{-1})^{-1}\nu_{\rm calc}(\alpha^6\ln\alpha^{-1}).$$

We note that the actual and expected percentages on lines three and four are in rather good agreement, indicating that the contributions in these orders are neither anomalously large nor small. Our estimate of $m\alpha^6$ contributions is made in the expectation that this trend will continue, but has no other basis in fact.

We list below the previous and present theoretical results and compare them with experiment, using the α of Eq. (5):

$$\nu_{\rm theor}(\text{Karplus and Klein}) = 2.033\,81\times10^5 \text{ MHz},$$
$$\nu_{\rm theor}(\text{present paper}) = 2.034\,27\times10^5 \text{ MHz},$$
$$\nu_{\rm expt}(1967) = 2.034\,03(12)\times10^5 \text{ MHz}. \quad (6)$$

One observes that, while the previous theoretical value was about two standard deviations below the experimental results, the contributions we obtain raise the theoretical value to two standard deviations above experiment. We note further that the estimated $m\alpha^6$ contributions could not bring the theoretical results to within one standard deviation of experiment.

Two recent calculations have eliminated disturbing discrepancies between experiment and

Table I. Theoretical contributions to positronium frequencies.

	Order	$\Delta\nu$ (10^5 MHz)	Percentage of contribution of last order: Actual	Expected
Schrödinger level (ionization frequency)	α^2	16 449.2	···	···
Triplet-singlet	α^4	2.043 86	0.012	0.005
Ground-state splitting	α^5	−0.010 05	0.491	0.73
	$\alpha^6\ln\alpha^{-1}$	0.000 46	4.58	3.6
	α^6(est)	±0.000 09	···	20

quantum electrodynamic (QED) theory, for the muon g-2 value[17] and for the hydrogen and deuterium Lamb shift.[18] Thus, apart from a possible discrepancy in the electron g-2 value,[16] the only remaining disagreement between theory and experiment in low-energy QED is the present one for positronium. This situation is all the more perplexing since, in contrast to hydrogen and the muon g-2 value, positronium presents a purely QED problem to this order. The calculations do not involve hadronic corrections or possible unexpected leptonic contributions. We therefore suggest that further computations of contributions to order $m\alpha^6 \ln\alpha^{-1}$ be carried out independently.

A detailed presentation of our calculation is in preparation.

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PAULI EXCITATION OF ATOMS IN COLLISION

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Experimental cross sections are reported for the ionization of K shells of Al in collision with N, O, and Ar (in the energy range 100-300 keV); of Ne with C, Ne, and Al (100-300 keV); and of Al with Ne (0.1-3.2 MeV). They are some 10^3 to 10^5 times larger than the cross sections one predicts for Coulomb excitation of K-shell electrons by swift charged particles. The cross sections are determined by the exchange forces set up in the overlapping electron clouds of atoms in collision. This process is referred to as Pauli excitation.

Recent progress in the study of the removal of inner-shell electrons of atoms by swift charged particles through measurements of characteristic x-ray yields have brought detailed understanding of the underlying Coulomb excitation process. One finds agreement with the ionization cross sections derived in the Born approximation[1] if the deflection of the incoming particle in the field of the target nucleus is taken into account, and if one incorporates the binding of the target electrons to the exciting particle.[2,3]

This note reports data on cross sections for the ionization of K shells by swift heavy atoms.[4] In comparison with the Coulomb-excitation cross sections, the cross sections are enormous—in fact, some 10^3 to 10^5 times larger. We attribute the cross sections to the exchange forces set up during collision by the Pauli exclusion principle in the overlapping electron clouds of the interpenetrating atoms. It forces the electrons into transient quasimolecular configurations leaving the atoms, on separation, in excited states. We refer to this process as the Pauli excitation of atoms in collision.