Positronium-ion decay

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We present a precise theoretical prediction for the decay width of the bound state of two electrons and a positron (a negative positronium ion), \( \Gamma(Ps^-) = 2.087\,085(12) \text{ ns} \). We include \( O(\alpha^2) \) effects of hard virtual photons as well as soft corrections to the wave function and the decay amplitude. An outcome of a large-scale variational calculation, this is the first result for second-order corrections to a decay of a three-particle bound state. It will be tested experimentally in the new positronium-ion facility in Garching in Germany.

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Positronium ion (\( Ps^- \)), consisting of two electrons and a positron, is the only known three-body bound state free from nucleons. Its existence was predicted by Wheeler in 1946 [1] and confirmed experimentally by Mills in 1981 [2]. Only the ground state is stable against a dissociation into positronium and an electron (see [3] for an extensive review of its properties and references). Electron-positron annihilation limits the \( Ps^- \) lifetime to about half a nanosecond, as first reported in [4]. Here we determine relativistic and radiative corrections to the annihilation in a three-body bound state and predict the \( Ps^- \) decay rate with a 6 parts per million precision,

\[
\Gamma(Ps^-) = 2.087\,085(12) \text{ ns}^{-1}.
\]

What makes the \( Ps^- \) ion particularly interesting is that its theory is very clean, albeit somewhat technically challenging. With a very good accuracy all but electromagnetic interactions in \( Ps^- \) can be neglected. Also the charge distribution of constituents is well known (point-like), unlike in atoms and ions containing nuclei. Quantum electrodynamics (QED) suffices to describe all properties of \( Ps^- \).

On the other hand, \( Ps^- \) is a three-body system and thus its wave function is not known analytically even in the non-relativistic approximation. This complicates theoretical investigations but also provides an opportunity to develop and test advanced computational techniques. Those new methods are important for other systems such as the hydrogen ion, the molecule \( H^+\,e^-\,e^- \), and the helium atom.

FIG. 1: The main decay channel of \( Ps^- \) (a), and an example of a correction to it, the three-photon annihilation (b).

The \( e^+e^- \) annihilation proceeds fastest when the pair is in a spin-singlet state, like para-positronium (pPs), in which case two photons can be produced (see Fig. 1(a)). If the pair is a spin triplet, like ortho-positronium (oPs), the decay results in an odd number of photons, Fig. 1(b). Interestingly, unlike ortho-positronium, \( Ps^- \) can also decay into a single photon. However, this channel is very rare [5, 6]: all three constituents have to overlap to transfer momentum to the non-annihilating electron. The three-photon decay is much more likely, but still much slower than the spin-singlet two-photon process.

The spatial wave function of \( Ps^- \) is symmetric with respect to the two electrons. For the total wave function to be antisymmetric, the two electrons must be in the spin-singlet state. It is convenient to think of \( Ps^- \) as consisting of a positronium core and a loosely bound electron [7]. This picture reveals the main features of the \( Ps^- \) lifetime. When \( e^+ \) meets one of the \( e^- \), the odds are about one in four that their spins form a singlet. Thus \( Ps^- \) lives about four times longer than pPs.

A variational determination of the \( Ps^- \) wave function [7] confirms this elegant argument. Furthermore, if this decay is so similar to that of pPs, the same \( O(\alpha) \) corrections apply [8]. In the same order, also the three-photon annihilation must be
accounted for \([9]\). Together, this led to the theoretical prediction for the \(\Ps^-\) decay width \([7]\),
\[
\Gamma_{\text{th}}^{1983} = 2.086(6) \text{ ns}^{-1},
\]
where the size of the \(\mathcal{O}(\alpha)\) corrections was used to estimate the uncertainty \([10]\) (see also \([11,12,13]\)).

Recent measurement \([10]\) agrees with this prediction and approaches its precision, \(\Gamma_{\text{exp}} = 2.089(15) \text{ ns}^{-1}\). It is anticipated that the new intense source of positrons at the Garching reactor FRM-II will be used to decrease the experimental error by a factor of 4 or 5, below the uncertainty in Eq. (2).

Motivated by this effort, we undertook to improve the theoretical precision by determining all \(\mathcal{O}(\alpha^2)\) effects. \(\Ps^-\), a non-relativistic bound state, is well described by the Schrödinger equation. Its leading-order decay rate is
\[
\Gamma_0 = 2\pi m_e \alpha^5 \langle \delta^3(r_{12}) \rangle,
\]
where \(m_e\) is the electron mass, \(r_{12}\) is the distance between the positron and the electron which annihilates, and the mean value refers to the ground state \(\Ps^-\) wave function
\[
\Psi = \psi(r_{12}, r_{13}, r_{23}) \chi(1, 2, 3), \quad \chi = \frac{\sqrt{2}}{\sqrt{2}}.
\]

Throughout this paper we use \(1/\alpha m_e, \alpha m_e, \text{ and } \alpha^2 m_e\) as units of length, momentum, and energy (we also set \(c = \hbar = 1\), except in the last Eq. (23)). Thus, \(\langle \delta^3(r_{12}) \rangle\) in Eq. (3), as well as all mean values to follow, are dimensionless.

Relativistic effects, spin of the electron, and short-distance exchanges of photons with a virtuality \(\mathcal{O}(m_e)\) are not accounted for by the Schrödinger equation, which includes only Coulomb potentials among the three constituents. Like in other non-relativistic systems \([14]\), these additional effects can be treated as perturbations and organized in a series in \(\alpha\),
\[
\Gamma = \Gamma_0 \left[ 1 + \alpha A + \alpha^2 \left( 2 \ln \frac{1}{\alpha} + B \right) - \frac{3\alpha^3}{2\pi} \ln^2 \frac{1}{\alpha} + \ldots \right].
\]
The first-order correction \(A\), already discussed, includes corrections to the two- and three-photon channels,
\[
A \equiv A^{2\gamma} + A^{3\gamma}, \quad A^{2\gamma} = \frac{\pi}{4} - \frac{5}{\pi}, \quad A^{3\gamma} = \frac{4\pi}{3} - \frac{12}{\pi}.
\]
Some authors (e.g. \([7]\)) hint at additional \(\mathcal{O}(\alpha)\) effects but in our opinion none other exist at this order.

In the next order, four photons contribute \([15]\), corrections \(\mathcal{O}(\alpha)\) must be included in the three-photon decay \([16,17]\), and \(\mathcal{O}(\alpha^2)\) in the two-photon decay \([18,19,20]\).

\[
B = B^{4\gamma} + B^{3\gamma} + B^{2\gamma}.
\]
The last term is the focus of this paper. It is a sum of several effects: square \(B_{\text{squared}}\) of the \(\mathcal{O}(\alpha)\) correction \(A^{2\gamma}\); hard-photon corrections \(B_{\text{hard}}\) to the \(e^+e^- \rightarrow \gamma\gamma\) process; and soft corrections to the annihilation amplitude \(B_{\text{aa}}\) and the wave function \(B_{\text{wf}}\):
\[
B^{2\gamma} = B_{\text{squared}} + B_{\text{hard}} + B_{\text{aa}} + B_{\text{wf}},
\]
\[
B_{\text{squared}} = \left( \frac{5}{2\pi} - \frac{\pi}{8} \right)^2,
\]
\[
B_{\text{hard}} = B_{\text{hard}}^{\text{fin}} - \frac{1}{2\epsilon}, \quad B_{\text{hard}}^{\text{fin}} = -\frac{4.06(30)}{\pi^2},
\]
\[
B_{\text{aa}} = \frac{1}{3},
\]

All corrections which affect only the annihilation amplitude have already been computed in the context of the pPs decay. Since they do not depend on the particular bound state, they apply to the present analysis without changes.

The correction to the wave function \(B_{\text{wf}}\), sensitive to the three-body dynamics, is the most challenging. As we will see below, it is divergent and cancels the divergence in \(B_{\text{hard}}\). The term \(-2\alpha^2 \ln \epsilon\) in Eq. (5) is a remnant of those divergences. In order to regularize divergences, we work in \(d = 3 - 2\epsilon\) spatial dimensions. Thus, the non-relativistic Coulomb Hamiltonian becomes
\[
H_0 = \sum_a \frac{\hat{p}_a^2}{2} + V,
\]
\[
V \equiv -\left[ \frac{1}{r_{12}} \right]_\epsilon - \left[ \frac{1}{r_{13}} \right]_\epsilon + \left[ \frac{1}{r_{23}} \right]_\epsilon \equiv \sum_{a<b} z_{ab} \left[ \frac{1}{r_{ab}} \right]_\epsilon,
\]
\[
\left[ \frac{1}{r} \right]_\epsilon \equiv \frac{\pi^{\epsilon-\frac{1}{2}} \Gamma \left( \frac{1}{2} - \epsilon \right)}{\Gamma^{1-2\epsilon}}.
\]
where \( \vec{p}_a, \vec{r}_{ab} \equiv \vec{r}_a - \vec{r}_b \) are momenta and relative distances of the positron 1 and electrons 2, 3.

The wave function correction arises due to relativistic effects, which are treated as a perturbation and described by the Breit Hamiltonian,

\[
H^{(4)} = \alpha^2 \left( H_1^{(4)} + \sum_{a<b} H_{2ab}^{(4)} \right)
\]

\[
H_1^{(4)} = -\sum_a \frac{p_a^2}{8} - \sum_{a<b} z_{ab} \left\{ \pi \delta^d(r_{ab}) + \frac{1}{2} \rho_a \left[ \frac{1}{r_{ab}} \right] \left( \delta^3 + (d-2) \frac{r_{ab}^2}{r_{ab}} \right) \rho_b \right\}
\]

\[
H_{2ab}^{(4)} = \frac{\pi z_{ab}}{4d} \left[ \sigma_i^a, \sigma_i^b \right] \delta^d(r_{ab})
\]

where the Pauli matrices are labeled with the number of the fermion they are acting on. It is convenient to evaluate separately the spin-independent part \( H_1^{(4)} \), and the spin-dependent part \( H_{2ab}^{(4)} \), \( B_{\text{ef}} \equiv B_{H1} + B_{H2} + \frac{1}{2\epsilon} \).

The effect of this perturbation is the following replacement in the formula for the decay rate, Eq. (3).

\[
\langle \delta^3(r_{12}) \rangle \rightarrow 2 \left( \frac{\delta^d(r_{12})}{(E-H_0)} \right) H^{(4)} \equiv \alpha^2 \left( B_{H1} + B_{H2} + \frac{1}{2\epsilon} \right) \langle \delta^3(r_{12}) \rangle.
\]

Here \( \frac{1}{(E-H_0)} \) is the Green’s function of the lowest-order Schrödinger equation and the prime indicates the exclusion of the ground state. The appearance of divergences is the main obstacle in the evaluation of this correction. They originate from \( r_{12} \to 0 \) (ultraviolet limit), where the Breit Hamiltonian is not a valid description of the dynamics. Indeed, when one accounts for the hard photons, Eq. (9), divergences cancel.

In analogy with the earlier work on positronium and helium [21, 22, 23, 24], we rewrite the matrix element in Eq. (15) such that the divergences appear only in the coefficient of one operator, namely \( \delta^d(r_{12}) \). To this end, we rewrite [24] the delta-function as

\[
4\pi \delta^d(r_{12}) = 4\pi \tilde{\delta}^d(r_{12}) + \left\{ H_0 - E, \left[ \frac{1}{r_{12}} \right] \right\}.
\]

This equation implicitly defines \( \tilde{\delta}^d \), less singular than \( \delta^d \). The most singular part is in the anticommutator in the second term. This term cancels the Green’s function, \( (E-H_0) \frac{1}{(E-H_0)} = I - |\Psi \rangle \langle \Psi| \), where \( I \) is the identity operator. Hence, divergences appear only in first-order elements and are easier to extract.

In the spin-independent part we find

\[
2\pi \langle \delta^3(r_{12}) \rangle \left( B_{H1} + \frac{1}{4\epsilon} \right) = 4\pi \delta^d(r_{12}) \frac{1}{(E-H_0)} H_1^{(4)} = \frac{1}{4} \sum_{i=1}^{21} v_i + \frac{1}{E^2} v_1 v_{22} + v_{23} + \frac{\pi}{2\epsilon} \langle \delta^3(r_{12}) \rangle,
\]

from which we can determine the value of \( B_{H1} \) in terms of the ground-state mean values listed in Table II. Among them, the regularized cubic operator is defined by Eq. (1.5) in Ref. [24].

In the spin-dependent part, the effect of Pauli matrices in \( H_{2ab}^{(4)} \), Eq. (14), is evaluated with the spin wave function in Eq. (4) and represented by constants \( A_{ab} \) for each pair of fermion lines: \( A_{12} = -2 - 6\epsilon, A_{13} = -A_{23} = -2 \). We keep \( \epsilon \) only in the coefficient of the divergent part. After this simplification of spins, we find

\[
2\pi \langle \delta^3(r_{12}) \rangle \left( B_{H2} + \frac{1}{4\epsilon} \right) = \sum_{a<b} \left\{ 4\pi \delta^d(r_{12}) \frac{1}{(E-H_0)} \pi A_{ab} \delta^d(r_{ab}) \right\}.
\]

In terms of the operators in Table II using the symmetry \( \vec{r}_2 \leftrightarrow \vec{r}_3 \) and the virial identity \( 2E = \langle V \rangle \), we get

\[
2\pi \langle \delta^3(r_{12}) \rangle B_{H2} = \frac{1}{2} (-v_7 - v_8 - v_{14} - v_{15} + v_{18}) + \frac{1}{6} (v_9 + v_{10}) + \frac{8E + 5}{4} v_{20} + \frac{1}{4} v_{21} + v_{24} + \frac{v_1}{E^2} (v_{25} - 2v_{20}).
\]

The numerical values in Table II are obtained with a variational method. The trial wave function is expanded in a 1000-element set of exponential functions [25]
where \( a, b, c \) are chosen randomly, with a homogeneous distribution, from two \( k \) sets defined by variational boundary conditions \( A_{1k} \leq a_{ki} \leq A_{2k}, B_{1k} \leq b_{ki} \leq B_{2k}, C_{1k} \leq c_{ki} \leq C_{2k} \). Two (or more) sets allow one to match the behavior of the wave function at various distance scales and improve accuracy. We found the non-relativistic energy value, \( E = -0.262005 070 232 980(1) \), that agrees with an even more accurate earlier result \([26]\). Previously obtained mean values of \( \langle \delta^3(r_{ab}) \rangle \) \([13, 27]\), and non-singular products of \( 1/r_{ab} \) \([13]\) are also confirmed. Finally, the mean value of the spin-independent part of the Breit Hamiltonian \( H_{1}^{(4)} \) agrees with Ref. \([27]\). Crucial for the decay is the mean value of the delta-function, obtained using the representation of Ref. \([28]\).

\[
\langle \delta^3(r_{12}) \rangle = 0.0207331980051(2).
\]  

This value agrees with the one found in \([27]\) and somewhat improves its accuracy.

For the new evaluation of the Ps\(^-\) decay rate we use \( \alpha = 1/137.03599911(46) \) and the atomic unit of time \( \alpha^2 m_e c^2/\hbar = 10^{17} \text s/2.418884326505(16) \) \([29]\). Our final result in Eq. \((1)\) is obtained using

\[
\Gamma(\text{Ps}^-) = 2\pi \frac{\alpha^5 m_e c^2}{\hbar} (1 + C) \langle \delta^3(r_{12}) \rangle,
\]  

where the correction \( C \) is given in Table \([\text{I}]\), and we use Eq. \((21)\). The last two corrections listed in Table \([\text{I}]\) refer to the third order in \( \alpha \). The leading quadratic logarithm was found in \([30]\) and is valid for positronium atoms as well as for the ion. The linear log (the last correction) has not yet been calculated for Ps\(^-\). However, it is known for pPs and oPs \([31, 32, 33]\). We expect its value for Ps\(^-\) to be close to that for pPs and use the latter as an estimate. We assign this correction a 100\% uncertainty, which also conservatively estimates non-logarithmic higher-order effects \([34]\).
Note that Ref. [27] includes a prediction of $\Gamma(Ps^- \rightarrow \gamma\gamma)$ with a seemingly higher precision than ours. That result, however, does not include any corrections beyond the tree level (this corresponds to setting $C = 0$ in our Eq. (22)) and its error estimate includes only the numerical uncertainty of the variational calculation in [27].  

Another experimentally interesting quantity is the branching ratio of the three-photon decay. We find

$$\text{BR}(Ps^- \rightarrow \gamma\gamma\gamma) \equiv \frac{\Gamma(Ps^- \rightarrow \gamma\gamma\gamma)}{\Gamma(Ps^-)} = \alpha \left[ A^3\gamma + \alpha \left( B^3\gamma - AA^3\gamma \right) - \frac{7}{3} A^3\gamma \alpha^2 \ln \frac{1}{\alpha} + \ldots \right] = 0.002 635 8(8).$$  

(23)  

The uncertainty is due to the unknown $O(\alpha^2)$ corrections to the decay $Ps^- \rightarrow \gamma\gamma\gamma$. Only the logarithmic term is known in this order [35], and we take half of its value to estimate the uncertainty.

The structure of corrections found in this study confirms the picture of $Ps^-$ as an electron loosely interacting with a positronium core [7]. The mean value in Eq. (21) is very close to that obtained with a neutral positronium, neglecting the second electron, $1/(16\pi) = 0.01989$. Also, in the sum of all effects in Table II there is a significant cancellation between the hard effects $B_{\text{hard}}$ and the soft ones $B_{\text{H1}} + B_{\text{H2}} + B_{\text{aa}}$, also observed in positronium [19]. It would be interesting to understand the origin of this cancellation, which for now remains an open question.

The accuracy we have obtained for the decay rate is 6 parts per million, about 500 times better than the previous best prediction, Eq. (4). Further progress in the theory of the $Ps^-$ decay requires the logarithmic term $O(\alpha^2 \ln \alpha)$ and improved hard corrections $O(\alpha^7)$. However, the accuracy obtained in the present paper is sufficient for the foreseeable future. It exceeds the anticipated accuracy of Garching measurements by about a factor of 200. We are thus prepared for the new data and are looking forward to this intriguing test of three-body bound-state QED.

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### Table II: Corrections to the width of $Ps^-$.  

| Correction | Value |
|------------|-------|
| $\alpha A^3\gamma$ | 0.002 693 245 |
| $\alpha A^2\gamma$ | -0.005 882 770 |
| $-2\alpha^2 \ln \alpha$ | 0.000 524 019 |
| $\alpha^2 B^4\gamma$ | 0.000 001 480 |
| $\alpha^2 B^3\gamma$ | -0.000 064 352 |
| $\alpha^2 B_{\text{aa}}$ | 0.000 177 500 |
| $\alpha^2 B_{\text{H1}}$ | 0.000 078 366 |
| $3\alpha^3 \ln^2 \alpha/(2\pi)$ | -0.000 004 491 |
| $2.5(2.5)\alpha^3 \ln \alpha$ | -0.000 004 8(48) |
| Total $C$ | -0.002 729 0(59) |

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