Positronium hydride decay into proton, electron, and one or zero photons

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Decay rates of the positronium hydride PsH, a bound state of a proton, a positron, and two electrons, are determined for two rare channels, $PsH \rightarrow p^+e^-\gamma$ and $PsH \rightarrow p^+e^-$. Previous studies overestimated these rates by factors of about 2 and 700, respectively. We explain the physics underlying these wrong predictions. We confirm a range of static PsH properties, including the nonrelativistic ground-state energy, expectation values of interparticle distances and their powers, and the three- and four-particle coalescence probabilities, using a variational method in the Gaussian basis.

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I. INTRODUCTION

Positronium hydride (PsH) consists of a proton p^+ , a positron e^+ , and two electrons e^- . Stable with respect to autoionization, it decays due to electron-positron annihilation. Similar to the case of the positronium ion (Ps⁻), its two electrons form a spin singlet. When the positron and one of the electrons meet, they can form a spin singlet or a triplet. Their annihilation can lead to final states with any number of photons, even or odd. Here we calculate the rates of decays that result in one or no photons, as well as an unbound electron and proton. Previously, these decay rates were only estimated, and we explain why those estimates were incorrect. The key issue is the role of the proton in influencing the $e^+e^$ annihilation.

In addition, we reevaluate the wave function of PsH using the variational method with a Gaussian basis. To test it, we calculate the nonrelativistic ground-state energy, mean interparticle distances, and, most importantly for our purposes, probabilities of coalescence of $e^+e^-e^-$ and of $p^+e^+e^-e^-$. We confirm the values of these quantities found in Ref. [1].

The motivation for this work is twofold. First, PsH is to a good approximation governed by quantum electrodynamics (QED), with only tiny corrections due to the structure of the proton (which are neglected in our work). QED systems can serve as models for more complicated phenomena like tetraquarks. Their properties should therefore be known with good accuracy, and in particular it is worthwhile to correct previously published estimates. Second, there is certain experimental interest in the detection of PsH [2]. It is important to have clarity about its branching ratios at least with orderof-magnitude accuracy.

The paper is organized as follows: In Sec. II we put our study in the context of previous work on PsH. In Sec. III we discuss its Hamiltonian and wave function. Section IV focuses on the decay $PsH \rightarrow p^+e^-\gamma$, and Sec. V on $PsH \rightarrow p^+e^-$. We conclude by comparing our results with previous literature in Sec. VI.

We use such units that $\hbar = c = \epsilon_0 = 1$, except for the expectation values of operators computed with the variational wave function of PsH, given in atomic units, as explained in Sec. III. We denote the electron mass by *m* and the proton mass by *M*. Unless indicated otherwise, we neglect the binding energy of PsH in comparison with *m* and treat its constituents as stationary particles, neglecting their relative motion. Corrections to this approximation are suppressed by the fine-structure constant $\alpha \simeq 1/137$.

II. BRIEF HISTORY OF PsH

In their pioneering works, Wheeler [3] and Hylleraas and Ore [4] studied small exotic molecules where one or more nuclei are replaced by positrons. Ore [5] established the stability of the PsH ground state. Since then, much theoretical work has been done on the energy of ground, metastable, and resonant states and on other properties of this system (see, for example, Refs. [6–20], where further references can be found).

Experimental efforts to produce and detect this system have also been made. Pareja *et al.* [21] first reported the existence of such a bound state in a condensed phase. Further evidence was provided by Schrader *et al.* [22] in positron-methane collisions,

$$e^+ + \mathrm{CH}_4 \to \mathrm{CH}_3^+ + \mathrm{PsH},\tag{1}$$

with an estimated binding energy, $E_b = -1.1 \pm 0.2$ eV, in line with most theoretical predictions.

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PsH is a special case of a Coulombic system, positioned between the hydrogen molecule H_2 and dipositronium Ps_2 , in which both nuclei are replaced with positrons. Since a positron's motion cannot be considered as slow, PsH is an essentially four-body system.

On the theoretical side, exotic systems containing antimatter serve to test various quantum-mechanical methods. Over the years, the accuracy of theoretical calculations in PsH has improved thanks to advances in computational techniques and increased hardware power. Using variational methods to obtain accurate wave functions, most of the studies performed for the ground-state energy of such a system are nonrelativistic; relativistic effects have been calculated by Yan and Ho [23] and by Bubin and Varga [1].

An interesting problem is the study of electron-positron annihilation in PsH producing zero, one, two, and in general *n* photons. What makes it more interesting is that the electron and proton can either be free or form a bound hydrogen state. References [24–26] considered both bound and unbound final states. In the case of unbound electron and p^+ final states, estimates were given for the two-photon annihilation rate $\Gamma_{2\gamma} = \Gamma(\text{PsH} \rightarrow p^+e^-\gamma\gamma)$, the dominant process. The rate of annihilation into three or more photons ($\Gamma_{n\gamma}$, $n \ge 3$) can be found using $\Gamma_{2\gamma}$ and the rate of the $n\gamma$ decay in a positronium atom. This is the subject of Ferrante relations [27], justified in [28].

Decays with one or no photons have been estimated using analogous Ps^- and Ps_2 results [28–30] in the absence of a dedicated QED calculation for PsH. Filling this gap is the main motivation of this paper.

III. VARIATIONAL DETERMINATION OF PROPERTIES OF PsH

A. PsH wave function and Hamiltonian

We label coordinates of the proton with 1, positron with 2, and electrons with 3 and 4. The PsH wave function is a product of spatial and spin parts, antisymmetrized with respect to permuting the electrons,

$$\psi = \chi_{\uparrow}^2 (\chi_{\downarrow}^3 \chi_{\uparrow}^4 - \chi_{\uparrow}^3 \chi_{\downarrow}^4) (1 + P_{34}) \phi_S, \qquad (2)$$

where χ 's denote spin states, P_{34} is the permutation operator of the electrons, and ϕ_S is the *S*-wave spatial wave function. In the Gaussian basis [31], that spatial part is written as

$$\phi_S = \sum_{i=1}^N c_i^S \exp\left[-\sum_{a < b} w_{ab}^{iS} r_{ab}^2\right],\tag{3}$$

where w_{ab} are real coefficients and N is the number of trial functions (basis size). Factors of $1/\sqrt{2}$ from the permutation operator and $1/\sqrt{4\pi}$ from the S-state wave function are absorbed in the normalization of linear coefficients c_i^S .

The proton, much heavier than the remaining constituents, is sometimes treated as a static source of the electric field [32]. In our approach, we follow the analogy with dipositronium [31] and include the motion of all four bodies. However, we neglect the magnetic moment of the proton throughout this paper so that the spin of the positron is the total angular

momentum of PsH, a constant. The Coulomb Hamiltonian is

$$\hat{H} = \sum_{i=1}^{4} \frac{\hat{p}_i^2}{2m_i} + \sum_{i < j} V(r_{ij})$$

= $\frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + \frac{\hat{p}_3^2}{2m_3} + \frac{\hat{p}_4^2}{2m_4} + \alpha \sum_{i < j} \frac{z_i z_j}{r_{ij}},$ (4)

where z_i equals -1 for e^- and +1 for e^+ and p^+ . Electron and positron masses are denoted by $m_2 = m_3 = m_4 \equiv m$. In atomic units (a.u.), we set m = 1 and $m_1 = M \simeq 1836$.

Let \vec{A}_i denote the absolute coordinates and \vec{r}_{ij} the relative coordinates. The interparticle distances are $r_{ij} = \sqrt{(\vec{A}_i - \vec{A}_j)^2}$. In terms of these coordinates, the Hamiltonian (4) becomes

$$\begin{aligned} \hat{H} &= -\frac{1}{2\mu_{12}} \left[\vec{\nabla}_{\vec{r}_{12}}^2 + \vec{\nabla}_{\vec{r}_{13}}^2 + \vec{\nabla}_{\vec{r}_{14}}^2 \right] \\ &- \frac{1}{m_1} \left[\vec{\nabla}_{\vec{r}_{12}} \cdot \vec{\nabla}_{\vec{r}_{13}} + \vec{\nabla}_{\vec{r}_{12}} \cdot \vec{\nabla}_{\vec{r}_{14}} + \vec{\nabla}_{\vec{r}_{13}} \cdot \vec{\nabla}_{\vec{r}_{14}} \right] \\ &+ \alpha \left[\frac{z_1 z_2}{r_{12}} + \frac{z_3 z_4}{r_{34}} + \frac{z_1 z_3}{r_{13}} + \frac{z_1 z_4}{r_{14}} + \frac{z_2 z_3}{r_{23}} + \frac{z_2 z_4}{r_{24}} \right], \tag{5}$$

where $\mu_{ij} = \frac{m_i m_j}{m_i + m_j}$ is the reduced mass, and in our case $\mu_{12} = \mu_{13} = \mu_{14}$. Translating from absolute to relative coordinates, we have ignored the kinetic energy of the center-of-mass motion of the PsH system.

The expectation value of the Hamiltonian with the wave function in Eq. (3) approximates the ground-state energy in terms of six exponents w_{ab}^{iS} . These six parameters are determined, for each of the N elements of the basis, following the optimization method described in [31]. The results for a range of parameters of the PsH system are given in Table I along with the corresponding values calculated in Ref. [1]. We find good agreement, especially for the nonrelativistic ground-state energy $\langle \hat{H} \rangle$. The binding energy (dissociation energy) is (in atomic units, taking $\alpha^2 mc^2$ as the unit energy)

$$E_b = -\langle \hat{H} \rangle + E^{\rm H} + E^{\rm Ps}$$

= $-\langle \hat{H} \rangle - \frac{3}{4} \text{ a.u.},$ (6)

where $\langle \hat{H} \rangle$ is given in Table I, and the ground-state energies of hydrogen and positronium are $-\frac{1}{2}$ and $-\frac{1}{4}$ a.u., respectively. The results we will use in Secs. IV and V are

$$\left< \delta_{e^+e_3^-} \delta_{e_3^-e_4^-} \right> = 3.73(2) \times 10^{-4},$$
 (7)

$$\langle \delta_{p^+e^+} \delta_{p^+e_3^-} \delta_{e^+e_4^-} \rangle = 1.85(1) \times 10^{-4}.$$
 (8)

The central values are arithmetic means of the results in Ref. [1] and ours. Their differences are used as error estimates. The reliability of our wave function is discussed in the following section.

B. Accuracy of the variational wave function

To check the accuracy of the variational wave function, we use the so-called virial factor,

$$\chi = \left| 1 + \frac{2\langle T \rangle}{\langle V \rangle} \right|,\tag{9}$$

$\langle r_{p^+e^+} \rangle$ 3.663 50 3.663 47	$\langle r_{e^+e^-} \rangle$ 3.481 18 3.481 16	$\langle r_{p^+e^-} \rangle$ 2.313 16 2.313 15	$\langle r_{e^-e^-} \rangle$ 3.5770 3.5770	$\langle r_{p^+e^+}^2 \rangle$ 16.272 16.272
$\langle r_{e^+e^-}^2 \rangle$ 15.593 54 15.593 22	$\langle r_{p^+e^-}^2 \rangle$ 7.824 79 7.824 54	$\langle r_{e^-e^-}^2 \rangle$ 15.895 94 15.895 43	$\langle 1/r_{p^+e^+}^2 \rangle$ 0.1720 0.1720	$\begin{array}{c} \langle 1/r_{e^+e^-}^2 \rangle \\ 0.349 \\ 0.349 \end{array}$
$\langle 1/r_{p^+e^-}^2 \rangle$ 1.205 65 1.205 62	$\langle 1/r_{e^-e^-}^2 \rangle$ 0.213 65 0.213 65	$\langle 1/r_{p^+e^+} \rangle$ 0.347 30 0.347 30	$\langle 1/r_{e^+e^-} \rangle$ 0.418 43 0.418 43	$(1/r_{p^+e^-})$ 0.729 0.729
$\langle 1/r_{e^-e^-}\rangle$	$\langle T angle$	$\langle V \rangle$	$\langle \hat{H} \rangle$	$\begin{cases} \langle \delta_{e^+e_3^-} \delta_{e^+e_4^-} \rangle \\ \equiv \langle \delta_{e^+e_3^-} \delta_{e_3^-e_4^-} \rangle \\ 3.7147 \times 10^{-4} \end{cases}$
0.370 33	0.788 87	-1.577 74	-0.78887 -0.78887	3.7364×10^{-4}
$\begin{cases} \langle \delta_{p^+e^+} \delta_{p^+e^-} \rangle \\ \equiv \langle \delta_{p^+e^+} \delta_{e^+e^-} \rangle \\ 8.6 \times 10^{-4} \\ 9.9 \times 10^{-4} \end{cases}$	$\langle \delta_{p^+e^+} \delta_{e_3^-e_4^-} \rangle$ 3.16×10 ⁻⁵ 2.12×10 ⁻⁵	$\langle \delta_{p^+e_3^-} \delta_{e^+e_4^-} \rangle$ 6.32×10 ⁻³ 6.00×10 ⁻³	$\langle \delta_{p^+e_3^-} \delta_{p^+e_4^-} \rangle$ 7.5334×10^{-3} 7.2097×10^{-3}	$ \begin{split} & \langle \delta_{p^+e^+} \delta_{p^+e_3^-} \delta_{e^+e_4^-} \rangle \\ & 1.9038 \times 10^{-4} \\ & 1.8018 \times 10^{-4} \end{split} $
	$\begin{array}{c} 3.663\ 50\\ 3.663\ 47\\ \langle r_{e^+e^-}^2 \rangle\\ 15.593\ 54\\ 15.593\ 22\\ \langle 1/r_{p^+e^-}^2 \rangle\\ 1.205\ 65\\ 1.205\ 62\\ \langle 1/r_{e^-e^-} \rangle\\ 0.370\ 33\\ 0.370\ 33\\ \{ \langle \delta_{p^+e^+} \delta_{p^+e^-} \rangle\\ \equiv \langle \delta_{p^+e^+} \delta_{e^+e^-} \rangle \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

TABLE I. Values of physical parameters for the PsH calculated using Gaussian wave functions, compared with results of Ref. [1]. All values are given in atomic units where the unit of length is the Bohr radius $\hbar/(\alpha mc)$. The basis size is always 1000.

where $\langle T \rangle$ and $\langle V \rangle$ are the expectation values of kinetic and potential energies, respectively. For an exact wave function, this parameter vanishes. We thus expect that it should be close to zero for a reliable wave function.

For the size of the basis N = 1000, expectation values of various operators are presented in Table I. In particular, $\langle T \rangle = 0.788\,87$ and $\langle V \rangle = -1.577\,74$, giving $\chi = 0$. Varying the last digits by one unit gives $\chi \simeq 10^{-5}$. This gives us confidence in our wave function.

This check, together with the agreement we find with Ref. [1] for all coalescence probabilities needed in our study, ensures the reliability of our results.

Another way of checking the wave function is Kato's cusp condition [33]; unfortunately, as we briefly explain below, it is not applicable in the case of the Gaussian trial functions we are employing. Kato's condition states that the exact wave function Ψ satisfies

$$\left. \frac{\partial \Psi}{\partial_{r_{ij}}} \right|_{r_{ij}=0} = q_i q_j \mu_{ij} = \nu_{ij}, \tag{10}$$

with q_i , q_j representing the charges of particles *i*, *j*, and μ_{ij} is their reduced mass. For a system of particles interacting through Coulomb potential, the average value of the cusp condition for a trial wave function ϕ is

$$\nu_{ij} = \frac{\left\langle \phi \left| \delta(r_{ij}) \frac{\partial}{\partial r_{ij}} \right| \phi \right\rangle}{\left\langle \phi \left| \delta(r_{ij}) \right| \phi \right\rangle}.$$
(11)

In the case of electron and positron, near the point of coalescence v_{ij} should be close to the exact value $-\frac{1}{2}$. Similarly, for an electron and a proton, it should be -1 (for an infinitely heavy proton). The cusp value for the PsH is calculated for various choices of trial wave function is (see Refs. [8,9,24,32]). However, for the PsH ground state, Gaussian wave functions give $\phi_S \approx \exp(-ar_{ij}^2)$ and the following

limit vanishes:

$$\lim_{r_i \to r_j} \delta(r_{ij}) \frac{\partial}{\partial r_{ij}} \phi_S = 0, \qquad (12)$$

making it impossible to calculate the cusp value [28].

We return to this point below when assigning a numerical uncertainty to our predictions.

IV. ONE-PHOTON DECAY PsH $\rightarrow p^+e^-\gamma$

Four types of diagrams can contribute to the decay PsH $\rightarrow p^+e^-\gamma$, as shown in Fig. 1. In all of them, an e^+e^- pair annihilates into one or two photons. One of the produced photons is absorbed by the spectator electron or by the proton.

We want to argue that the dominant (by far) contribution is provided by diagrams A and B in Fig. 1, where a photon is absorbed by the spectator electron. Diagrams C and D are strongly suppressed and can be neglected. Since PsH is weakly bound, its constituents' velocities are small and can be neglected. In that limit, the proton can be treated as a static source of Coulomb photons. In group C, the two-photon annihilation occurs only for a spin-singlet e^+e^- pair. The spinsinglet projector contains γ^5 [34], and, for the amplitude not to vanish, Dirac matrices $\gamma^{1,2,3}$ must be supplied by vertices and by the electron's propagator. Interaction with a Coulomb photon, coupled via γ^0 , does not contribute. Similarly, in group D, the matrix γ^0 has a zero matrix element between spinors of a positron and an electron at rest.

For this reason, it is sufficient to consider groups A and B, up to corrections suppressed by powers of α which are small and beyond the scope of this work. These two groups are the same as the diagrams responsible for the positronium ion decay Ps⁻ $\rightarrow e^{-\gamma}\gamma$, first evaluated in [35] and recently confirmed in [36]. The only difference is in the coalescence

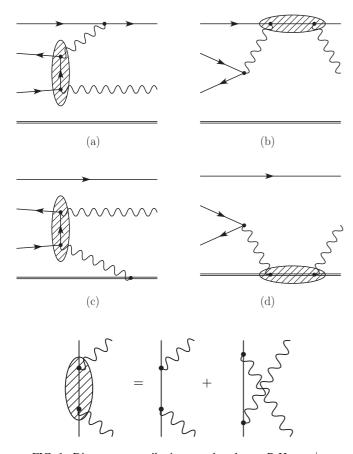


FIG. 1. Diagrams contributing to the decay $PsH \rightarrow p^+e^-\gamma$. Electrons and positrons are represented by solid straight lines and the proton by a double line. Blobs indicate two possible orderings of photon couplings.

probability of $e^-e^-e^+$, which is much larger in PsH than in the ion, thanks to the attraction of electrons to the proton.

When the ion Ps⁻ is isolated, we know that it is approximately a Ps atom accompanied by an electron far away [37]. In the presence of a proton, this configuration becomes more compact. If PsH resembles a hydrogen molecule, one may expect the two electrons to be predominantly between the proton and the positron, binding the system. It is reasonable to expect the probability of $e^-e^-e^+$ coalescence to scale like the inverse volume of the system, which we can estimate as proportional to $1/r_{e^-e^-}^-$, where $r_{e^-e^-}$ is the mean

distance between the electrons. Using numbers in Table I and those for the ion from Ref. [38], we get the volume ratio $[r(Ps^-)/r(PsH)]^3$ equal to about 13.6. This is consistent with the ratio of coalescence probabilities: for PsH, Eq. (7) gives $\langle \delta_{e^+e_3^-} \delta_{e_3^-e_4^-} \rangle = 3.73(2) \times 10^{-4}$, which is about 10 times larger than 0.358 75(2)×10⁻⁴ in the ion Ps⁻ [38]. This consistency among various estimates obtained with the variational approach is reassuring.

Finally, we obtain the one-photon decay rate by substituting the PsH value of $\langle \delta_{e^+e_3^-} \delta_{e_3^-e_4^-} \rangle$ into Kryuchkov's [35] result for the Ps⁻,

$$\Gamma(\text{PsH} \to p^+ e^- \gamma) = \frac{64\pi^2}{27} \alpha^9 m \left\langle \delta_{e^+ e_3^-} \delta_{e^+ e_4^-} \right\rangle = 0.398(12) \,\text{s}^{-1}.$$
(13)

We have quadrupled the error arising from the numerical evaluation of the coalescence probability to account for corrections of higher order in α . We have further increased the error estimate since our Gaussian trial functions cannot be tested for Kato's cusp condition, as discussed in Sec. III B.

V. ZERO-PHOTON DECAY PsH $\rightarrow p^+e^-$

PsH can also decay with only an electron and a proton in the final state, $PsH \rightarrow p^+e^-$, when photons produced in the e^+e^- annihilation are absorbed by surviving components of PsH (internal conversion). This channel is very suppressed because it requires all four constituent to coalesce, and also it is of a higher order in α . Its signature is a relativistic electron with energy of about 3m. Since our result for this decay differs from previous studies by orders of magnitude, we describe our calculation in detail. Diagrams contributing to the decay PsH $\rightarrow p^+e^-$ are shown in Fig. 2. They are divided into three groups A, B, and C, differing by the topology of the photon exchange. Working in the leading order in the velocities of the constituent particles, one can neglect groups B and C, by the same reasoning as at the beginning of Sec. IV.

We therefore evaluate only diagrams in group A, shown in Fig. 3. We frame the calculation as a decay of Ps⁻ in an external Coulomb field. Choosing the z axis along the polarization of the positron, we compute the amplitude of the electron emission along that axis. The electron emitted in that direction must be right-handed since it carries the spin of the initial state. The amplitude of emission at a nonzero polar angle θ will be multiplied by $\cos(\theta/2)$, resulting in

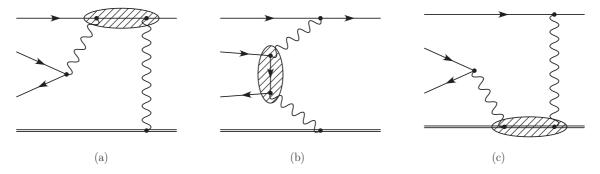


FIG. 2. Diagrams contributing to the decay PsH $\rightarrow p^+e^-$ with no photons in the final state. As in Fig. 1, blobs denote two orderings of photon couplings.

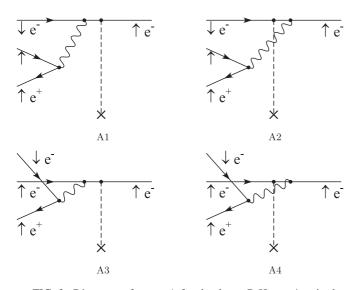


FIG. 3. Diagrams of group A for the decay $PsH \rightarrow p^+e^-$ in the limit of an infinitely massive proton. Dashed line denotes interaction with the Coulomb field of the proton.

a factor $\langle \cos^2(\theta/2) \rangle = 1/2$ in the decay rate. That factor is canceled when the rate of decay into a left-handed electron is included. [If daughter electrons' polarization is not observed, their angular distribution is isotropic because of $\cos^2(\theta/2) + \sin^2(\theta/2) = 1$.]

The daughter electron carries the rest energy of the initial state, $E_f = 3m$. For it to be on the mass shell, the Coulomb photon exchanged with the nucleus (dashed line in Fig. 3) must carry momentum $p_f = 2\sqrt{2m}$ in the *z* direction. Its propagator supplies a factor of $e/(8m^2)$ to the amplitude. The remaining factors for the amplitudes pictured in Fig. 3 are (amplitudes 3 and 4 contain a minus sign relative to 1, 2, due to permutation of fermion operators)

$$\mathcal{M}_{1} = \mathcal{M}_{2} = -\frac{e^{3}}{8\sqrt{2}m^{3}}, \quad \mathcal{M}_{3} = -\frac{e^{3}}{16\sqrt{2}m^{3}},$$
$$\mathcal{M}_{4} = \frac{3e^{3}}{16\sqrt{2}m^{3}}, \quad (14)$$

$$\mathcal{M} = \sqrt{2}(\mathcal{M}_1 + \mathcal{M}_2 + \mathcal{M}_3 + \mathcal{M}_4) = -\frac{e^3}{8m^3},$$
 (15)

where the factor of $\sqrt{2}$ arises from the electron spin-singlet wave function, $(\uparrow \downarrow - \downarrow \uparrow)/\sqrt{2}$: there are two equal contributions divided by $\sqrt{2}$. These results are obtained assuming free particles annihilating at rest, using the daughter electron's spinor $u_f^{\dagger} = (1 \ 0 \ 1/\sqrt{2} \ 0)$. To account for the binding, the amplitude is multiplied [36] by the PsH wave function at zero separation among the positron and electrons. The square of the amplitude is summed over the final states. The rate is a product of four factors: final-state normalization, amplitude squared, phase space, and the coalescence probability that includes 1/2! accounting for identical electrons,

$$\Gamma(\text{PsH} \to p^+ e^-) = \frac{1}{u_f^{\dagger} u_f} \left(\frac{e^4}{64m^5}\right)^2 \frac{4\pi p_f E_f}{(2\pi)^2} \frac{(\alpha m)^9 \langle \delta_{p+--} \rangle}{2!}$$
(16)

$$=\frac{\sqrt{2}}{8}\pi^{3}\alpha^{13}\langle\delta_{p+--}\rangle m, \qquad (17)$$

where $\langle \delta_{p+--} \rangle$ denotes $\langle \delta_{p^+e^+} \delta_{p^+e_3^-} \delta_{e^+e_4^-} \rangle = 1.85(1) \times 10^{-4}$ given in Eq. (8). Using this value, we get the rate

$$\Gamma(\text{PsH} \to p^+ e^-) = 1.31(10) \times 10^{-10} \text{ s}^{-1}.$$
 (18)

As in Eq. (13), we have increased the error estimate to account for the uncertainty in the Gaussian trial functions at coalescence points.

VI. CONCLUSIONS

We have determined the rates of two rare decays of the ground state of positronium hydride, and we confirmed a number of basic properties for this system using the variational principle with a Gaussian basis.

In the case of one-photon annihilation, $PsH \rightarrow p^+e^-\gamma$, where one of the photons produced in the e^+e^- annihilation can be absorbed either by the electron or by the proton, we have demonstrated that the proton contribution is negligible. When the electron absorbs the photon, the decay resembles that of the already extensively studied Ps^- ion. We find [see Eq. (13)]

$$\Gamma(\text{PsH} \to p^+ e^- \gamma) = 0.398(8) \,\text{s}^{-1}.$$
 (19)

The assigned error includes the spread of values of the coalescence probability, higher-order α corrections, and much smaller proton recoil effects. This result should be compared with previous estimates. Reference [28] assumed (incorrectly) that the contribution of the photon absorption by the proton "does not differ significantly from" that by the electron and thus they obtained a rate about twice as large as what we obtained, 0.8077 s⁻¹ (Table V in Ref. [28]). Similarly, Ref. [39] repeated the claim that absorptions by the electron and by the proton contribute approximately equally, and they obtained 0.787 501 s⁻¹ using a slightly different coalescence probability. We stress once again that the photon absorption by the proton is suppressed by the velocity of constituents of PsH, equivalent to a suppression by α .

The other decay channel we considered was the radiationless decay $PsH \rightarrow p^+e^-$ for whose rate we found in Eq. (18), $1.31(7) \times 10^{-10} \text{ s}^{-1}$. The previous estimate [28], $9.16 \times 10^{-8} \text{ s}^{-1}$, is larger by a factor of almost 700. That estimate was obtained by using the dipositronium Ps₂ result [Eq. (32) in Ref. [28]]. There are two problems with this reasoning. First, the Ps₂ formula used in Ref. [28] was incorrect even for Ps₂: it overestimated the zero-photon decay rate of Ps₂ by a factor of about 5.44 [36]. What about the remaining factor of 700/5.44 \simeq 130? The Ps₂ decay is quite different from that of PsH. The numerical coefficient in Ps₂ is $27\sqrt{3}/2 \simeq 23$ [36] instead of that in PsH being $\sqrt{2}/8 \simeq 0.18$ [see our Eq. (17)]. Their ratio is 23/0.18 \simeq 130, explaining the remaining discrepancy.

This large ratio has several sources: different symmetry factors, the proton not contributing in PsH, and, crucially, different particle virtualities. In the PsH decay, the emitted electron carries a large momentum with a magnitude of $\sqrt{8m}$. The propagator of the Coulomb photon supplying this

momentum introduces a large suppression factor. Just to illustrate how this leads to large numbers, consider the diagram similar to diagram B of Fig. 2 in the decay $Ps_2 \rightarrow e^+e^-$: the denominators in the propagators of the photons and of the virtual electron are, in units of $1/m^2$, -1/2, -1/2, 1/4, producing 1/16. Now consider denominators in Fig. 2, diagram A, for PsH $\rightarrow p^+e^-$: 1/4, 1/8, -1/8, giving -1/256. Rates involve squares of these products, favoring the Ps₂ rate by the relative factor of 256. This illustrates how the ratio of 130 of the Ps₂ and PsH rates is quite natural.

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