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New calculation of the properties of the positronium ion

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The positronium negative ion (Ps^-), the system composed of two electrons and a positron, has been reinvestigated theoretically. Using a Hylleraas wave function with two nonlinear parameters and more than 200 linear terms, we have obtained excellent values of binding energy and annihilation lifetime of the particle-stable $^1S^e$ ground state. In addition, we have examined the question of stability of the $^3P^e$ state discussed by Mills, and we agree with his conclusion that the state is probably not stable against breakup into $Ps(n=2)+e^-$. Improved limits on the critical "positron" mass for binding the $^3P^e$ state have also been obtained.

As a result, in part, of the recent elegant experimental work of Mills,[1,2] there has been a revival of interest in the simplest "polyelectron" system,[3] the positronium negative ion (Ps^-). Consisting of two electrons and a positron, this isotope of H^- has long been known[4] to be particle stable, decaying only by e^+-e^- annihilation into gamma rays. Mills has recently produced and detected this ion[1] and measured its lifetime,[2] while Ho has calculated with high accuracy its ground-state[5] and resonant-state[6] properties. In this paper we report some even more accurate results concerning the Ps^- ground state and confirm[7] the probable nonexistence of an excited state analogous to the known $^3P^e$ state in H^-.

In reduced rydberg units ($R_\mu=\mu/m_e$ Ry) the Hamiltonian of the system is

$$H_\rho=-\nabla_1^2-\nabla_2^2-\frac{2}{1+\rho}\vec{\nabla}_1\cdot\vec{\nabla}_2-\frac{2}{r_1}-\frac{2}{r_2}+\frac{2}{r_{12}}\ , \quad (1)$$

where the reduced mass $\mu=m_+m_-/(m_++m_-)$, $\rho=m_+/m_-$, and $\vec{r}_1$, $\vec{r}_2$ are the vectors from the positive particle to each of the identical negative particles in units of $(m_e/\mu)a_0$. (For generality, we allow the masses m_+, m_- to differ from m_e.) We take as trial function the generalized Hylleraas form

$$\Psi(\vec{r}_1,\vec{r}_2)=(\sin\theta_{12})^L\sum_{\substack{l\geq L,\\ m\geq L,\\ n\geq 0}} C_{lmn}[r_1^l r_2^m e^{-(\gamma r_1+\delta r_2)} +(1\leftrightarrow 2)]r_{12}^n \mathscr{D}_L^{0+}\ , \quad (2)$$

where $L=0,1$ for $^1S^e$ and $^3P^e$ states, respectively, and the $\mathscr{D}$ functions involve the symmetric Euler angles[8] describing the orientation in space of the vectors $\vec{r}_1$ and $\vec{r}_2$. We follow Ref. 8 in the reduction of H_ρ to an operator in r_1, r_2, and r_{12} only, after which the usual variational type of calculation can be carried out.

In Table I we show the convergence of our $^1S^e$ results under the restriction of setting the two nonlinear parameters equal ($\delta=\gamma$), while the more general case ($\delta\neq\gamma$) is shown in Table II. A considerable improvement in the energy is seen in the latter case; the optimum values for the two parameters differ by about a factor of 2. This reflects the basic structure of the Ps^- ground state which consists mainly of the Ps atom plus a loosely bound electron. Our best value of the binding energy against breakup of Ps^- into $Ps+e^-$ is 0.024 010 113 Ry or 0.326 676 9(9) eV, where the quoted uncertainty is due to the error in converting rydberg units to electronvolts. This is greater by 4.4×10^{-6} eV than the previous best value calculated by Ho.[5] By extrapolation, we estimate the converged value of the energy to be $0.024\,010\,130\pm3\times10^{-9}$ Ry.

In Tables I and II we also show several other quantities. These include expectation values of $\delta(\vec{r}_i)$ and $\delta(\vec{r}_{12})$ and the two cusp quantities

$$\nu_i=\left\langle\delta(\vec{r}_i)\frac{\partial}{\partial r_i}\right\rangle\langle\delta(\vec{r}_i)\rangle^{-1}\ ,$$
$$\nu_{12}=\left\langle\delta(\vec{r}_{12})\frac{\partial}{\partial r_{12}}\right\rangle\langle\delta(\vec{r}_{12})\rangle^{-1}\ . \quad (3)$$

TABLE I. Convergence of $^1S^e$ results for $\delta=\gamma$. [The notation $A(-B)$ stands for $A\times10^{-B}$.]

Expansion length	$\gamma=\delta$	Binding energy (Ry)	$\delta(\vec{r}_i)$	$\delta(\vec{r}_{12})$	ν_i	ν_{12}	Γ ($nsec^{-1}$)
125	0.3585	0.024 009 788	0.020 722	1.715 1(−4)	−0.499 10	0.497 11	2.0850
161	0.3700	0.024 010 026	0.020 732	1.713 6(−4)	−0.499 86	0.496 95	2.0860
203	0.3800	0.024 010 089	0.020 730	1.712 9(−4)	−0.499 64	0.497 40	2.0858

TABLE II. Convergence of $^1S^e$ results for $\delta \neq \gamma$.

Expansion length	γ	δ	Binding energy (Ry)	$\delta(\vec{r}_i)$	$\delta(\vec{r}_{12})$	ν_i	ν_{12}	Γ (nsec^{-1})
120	0.604	0.296	0.024 009 966	0.020 733	1.719 0(−4)	−0.500 00	0.493 47	2.0861
165	0.604	0.314	0.024 010 079	0.020 733	1.716 4(−4)	−0.499 99	0.494 41	2.0861
220	0.604	0.313	0.024 010 113	0.020 733	1.715 0(−4)	−0.500 00	0.495 08	2.0861

The cusp quantities test the accuracy of wave functions near points of coalescence, since $\nu_1 = \nu_2 = -\frac{1}{2}$ and $\nu_{12} = +\frac{1}{2}$ for exact solutions of the Schrödinger equation.[9] Our solutions are seen to be quite good, with ν_i lying closer to the exact value than ν_{12}. To a sufficient accuracy the Ps^- decay rate is

$$\Gamma = 2\pi\alpha^4(c/a_0)[1-\alpha(17/\pi - 19\pi/12)]\langle\delta(\vec{r}_1)\rangle$$
$$= 100.617\,4\langle\delta(\vec{r}_1)\rangle\ \mathrm{nsec}^{-1}\ , \qquad (4)$$

where the correction term proportional to α is due to the triplet lifetime[10] and the leading radiative correction to the singlet lifetime.[11] (There are some additional corrections of order α that have not yet been calculated.) Our theoretical value is in agreement with the measured[2] value $\Gamma = 2.09 \pm 0.09\ \mathrm{nsec}^{-1}$, although the experiment is not yet precise enough to test the theory critically. In fact, the crude picture of Ps^- as a loosely bound electron plus Ps discussed above leads to an estimated value of $\langle\delta(\vec{r}_1)\rangle = 1/16\pi$ or a rate of 2.0017 nsec^{-1}, still in agreement with experiment.

Mills[7] recognized that the existence of a $^3P^e$ state in Ps^- lying below the $n=2$ threshold of Ps would have very interesting experimental consequences: The state would be metastable against breakup since the process $Ps^-(^3P^e) \rightarrow Ps(^1S) + e^-$ is nonrelativistically forbidden, while the annihilation rate in p states is of order α^2 smaller than for s states.[12] Such a state is known[13] in H^-, but is very weakly bound; it lies only 9.5×10^{-3} eV below the $n=2$ threshold. Mills[7] showed, by use of variational wave function with up to 70 terms, that the state is probably not bound in Ps^-. Perhaps this should not be surprising since the ground state of Ps^- is bound by only about half as much as that of H^-. We have, nevertheless, recalculated the energy of the $^3P^e$ state in Ps^- using the trial function of Eq. (2) with $L=1$ and up to 120 terms and have failed to obtain an energy below $-\frac{1}{4}$ reduced rydbergs, the $n=2$ threshold. We tried to improve the convergence by adding long-range terms of several types,[14] but the improvement was not noteworthy.

Following Mills[7] we then varied the mass ratio ρ to bound the region in which the $^3P^e$ state is stable. In Table III we show the convergence for two cases: $\rho=17$, for which binding definitely occurs, and $\rho=16$, for which no binding was obtained. In Fig. 1, we plot the binding energy in reduced rydberg units versus ρ, showing that binding occurs[15] for all values of ρ except $0.4047 \leq \rho \leq 16.8$. The region for which binding does occur includes such interesting systems as H^-, $e^-\mu^+e^-$, H_2^+, and the muonic hydrogen molecular ions ($p\mu p$, $d\mu d$, $t\mu t$), but excludes Ps^-, for which $\rho=1$.

TABLE III. Convergence of $^3P^e$ binding energies $[E(n=2)-E]$ for two cases. Energies are in reduced rydbergs; $\rho = m_+/m_-$.

Expansion length	$\rho=17$	$\rho=16$
20	−1.950 52(−4)	−2.358 43(−4)
35	−6.744 6(−5)	−1.044 28(−4)
56	−1.810 4(−5)	−5.262 7(−5)
84	−1.021 (−6)	−3.461 9(−5)
120	+6.900 (−6)	−2.602 9(−5)

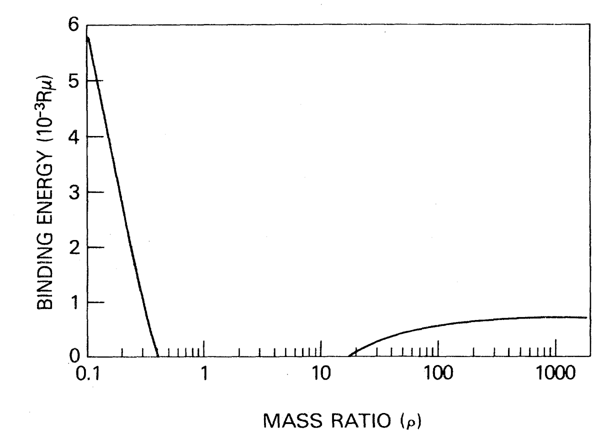

FIG. 1. Binding energy of $^3P^e$ state $[E(n=2)-E]$ in reduced rydbergs as a function of the mass ratio ρ.

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[15]Close to these limiting values of ρ, the effect of the long-range term of Ref. 14 is more important. Its inclusion reduces the upper limit from $\rho = 16.8$ to $\rho = 16.1$. In addition, an extrapolation from $N = 120$ to $N = \infty$ further reduces the upper limit to $\rho = 15.8$, but this is not rigorous.