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Brief Reports

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Probable nonexistence of a $^3P^e$ metastable excited state of the positronium negative ion

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The H^- ion is known to have a metastable $2p^2\,{}^3P^e$ triplet excited state. To see if an analog of this state is present in the positronium negative ion Ps^- the Coulomb binding energy E_b of the lowest-energy even-parity $L=1$ configuration of two identical-charge $-e$ fermions of mass m_1 plus one spinless particle of mass m_2 and charge $+e$ is calculated. We find a value of E_b below the $n=2$ level of the neutral atom for $0 \le m_2/M \le 0.17$ and $0.90 < m_2/M \le 1$, where $M=2m_1+m_2$ is the total mass of the ion. However, we cannot say that the $^3P^e$ state exists for Ps^-, where $m_2/M=\frac{1}{3}$.

The existence of a bound state of a positron and two electrons was predicted in 1946 by Wheeler[1] and was recently confirmed by observation.[2] It is interesting to ask whether this positronium negative ion Ps^- ($e^+e^-e^-$) has a metastable excited state analogous to the $2p^2\,{}^3P^e$ state of H^- predicted by Holøein and others.[3] Such a Ps^- state would have fine structure and would decay not by annihilation (there is no e^+e^- overlap in first order) but by a slow radiative transition to an autoionizing Ps^- configuration. We present here a calculation of the $^3P^e$ Coulomb binding energy of three particles which unfortunately does not show the existence of a metastable excited state for Ps^-.

While there are numerous calculations dealing with the ground-state[4] and autoionizing resonances[5] of Ps^-, these have dealt exclusively with states having zero total angular momentum. We may extend the usual Hylleraas[6] or Pekeris[7] calculation to our $^3P^e$ problem as follows. Neglecting the center-of-mass motion, the Hamiltonian for two identical fermions of mass m_1 and like charge interacting with an oppositely charged particle of mass m_2 is

$$H = -\frac{\hbar^2}{2\mu_1}\nabla_1^2 - \frac{\hbar^2}{2\mu_2}\nabla_2^2 + \frac{e^2}{u} - \frac{e^2}{s} - \frac{e^2}{t}, \quad (1)$$

where the problem has been reduced to a two-body problem[8]: μ_1 is the reduced mass of the two like particles relative to each other, $\mu_1 = m_1/2$; μ_2 is the reduced mass of the third particle relative to

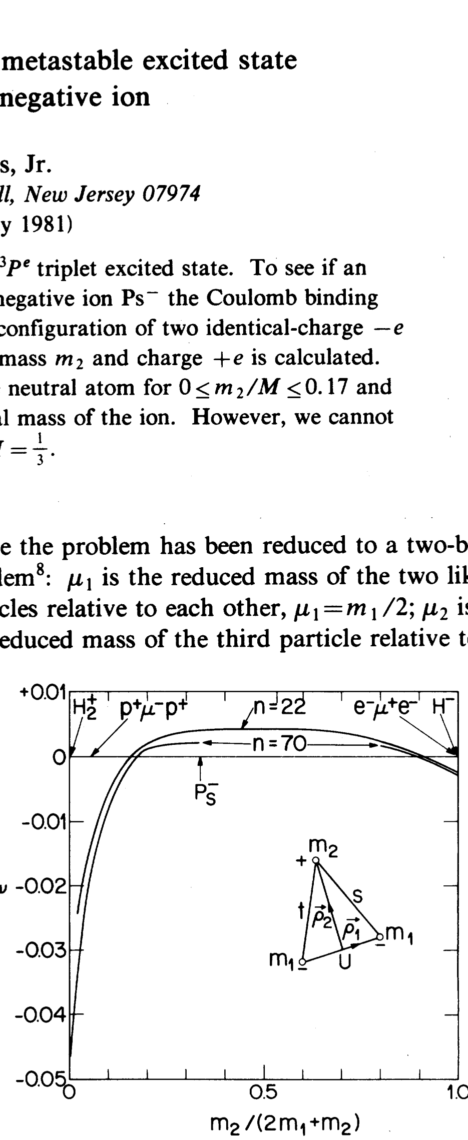

FIG. 1. Relative dissociation energy ϵ of the $^3P^e$ state of H^--like ions vs the relative mass m_2/M of the unlike particle. Positive values of ϵ show where the calculation is not sufficiently precise to give the free particle value $\epsilon=0$. The curves were calculated for $\Omega=4$ and 7 which means $n=22$ and 70 different terms were included. The inset shows the coordinates used to calculate binding energies of three charged particles.

the first two, $\mu_2=2m_1m_2/(2m_1+m_2)$; the reduced coordinates are the separation of the two identical particles $\vec{\rho}_1$, and the separation of the third particle from the center of mass of the identical pair $\vec{\rho}_2$, with ∇_1^2 and ∇_2^2 being the Laplacian for $\vec{\rho}_1$ and $\vec{\rho}_2$, respectively. As shown in Fig. 1, the separations between the three particles are $u=|\vec{\rho}_1|$, $s=|\vec{\rho}_2-\frac{1}{2}\vec{\rho}_1|$, and $t=|\vec{\rho}_2+\frac{1}{2}\vec{\rho}_1|$. A Hylleraas wave function for the $L=0$ ground state ($^1S^e$) is

$$\psi_S=\sum_{k,l,m} a_{klm}\psi_{klm}\ , \tag{2}$$

where the wave functions

$$\psi_{klm}=u^k(s^lt^me^{-(\alpha s+\beta t)}+s^mt^le^{-(\alpha t+\beta s)}) \tag{3}$$

are symmetric under $\vec{\rho}_1\rightarrow-\vec{\rho}_1$ as is required when the two identical fermions are in a relative singlet state. The Schrödinger equation $H\psi_S=E\psi_S$ becomes

$$\sum_{klm}(\psi_{k'l'm'},H\psi_{klm})a_{klm}=\sum_{klm}E(\psi_{k'l'm'},\psi_{klm})a_{klm}\ , \tag{4}$$

where the symbols $(\psi,A\psi')$ denote overlap integrals. We let i denote a certain combination of k, l, and m, and we let Ω be the largest value of $k+l+m$. Defining $H_{i'i}=(\psi_{k'l'm'},H\psi_{klm})$ and $A_{i'i}=(\psi_{k'l'm'},\psi_{klm})$ we have

$$\sum_{i'i}A^{-1}_{i''i'}H_{i'i}a_i=Ea_{i''}\ .$$

An upper limit on the ground-state binding energy is found by minimizing the lowest-energy eigenvalue of $A^{-1}H$ with respect to the parameters α and β.

The metastable triplet excited state in which we are interested has even parity and one unit of angular momentum ($^3P^e$). Thus, if its binding energy is below the $n=2$ state of the neutral atom, the $^3P^e$ state is stable with respect to emission of a particle. The only available final state is the even-parity $L=0$ ground state plus a free particle which must have $L=1$ and thus odd parity. Since the electromagnetic interaction conserves parity, such a transition will not be possible. Instead, a $^3P^e$ state bound below the $n=2$ threshold must first emit a photon before autoionizing.

A Hylleraas wave function for the $^3P^e$ state is obtained by multiplying a wave function with the symmetry of ψ_S by the axial vector $\vec{\rho}_1\times\vec{\rho}_2$ which has $L=1$ but is even under parity $(\vec{\rho}_1,\vec{\rho}_2)\rightarrow(-\vec{\rho}_1,-\vec{\rho}_2)$. The $m=0$ state wave function is thus

$$\psi_{^3P^e}=(\vec{\rho}_1\times\vec{\rho}_2\cdot\hat{z})\sum_{k,l,m}a'_{klm}\psi_{klm}\ . \tag{5}$$

This represents a triplet state because it is odd under $\vec{\rho}_1\rightarrow-\vec{\rho}_1$. Using Cartesian coordinates for $\vec{\rho}_1$ and $\vec{\rho}_2$ it is straighforward to show that $H(\vec{\rho}_1\times\vec{\rho}_2\cdot\hat{z})\psi_{klm}$ is a linear combination of other $(\vec{\rho}_1\times\vec{\rho}_2\cdot\hat{z})\psi_{klm}$'s. The overlap integrals are easily performed using Pekeris's[7] perimetric[9] coordinates. The matrix elements are then evaluated numerically and the lowest eigenvalue E_b of $A^{-1}H$ for a given choice of m_2/M, α/β, and Ω is minimized

TABLE I. Dissociation energies of the $^1S^e$ and $^3P^e$ states of various H^--like ions. The dissociation energy is the binding energy relative to the autoionization threshold. The number of terms in the present calculation is $n=70$. The total mass of the ion is $M=2m_1+m_2$.

Ion	Mass ratio m_2/M	Dissociation energies (eV) $^1S^e$	$^3P^e$
H_2^+	0.000 272 2	2.644[a]	0.162[e]
$p^+\mu^-p^+$	0.053 304	253.9[b]	12.35[e]
Ps^-	$\frac{1}{3}$	0.326 67[c]	
$e^-\mu^+e^-$	0.990 42	~0.7	0.008 59[e]
H^-	0.998 91	0.747[d]	0.009 65[f]
H^-			0.009 48[e]

[a]V. A. Johnson, Ref. 11.
[b]W. K. Wessel and P. Phillipson, Ref. 11.
[c]Y. K. Ho (unpublished).
[d]C. L. Pekeris, Ref. 7; A. A. Frost *et al.*, Ref. 4.
[e]Present results representing lower limits to the exact values.
[f]A. K. Bhatia, Ref. 3.

with respect to the parameter β. In Fig. 1 we plot the dissociation energy relative to the $n=2$ threshold,

$$\epsilon=[E(n=2)-E_b]/E(n=2)\ ,$$

for $\Omega=4$ and 7, for $\alpha/\beta=\frac{1}{4}$, and for $0<m_2/M_1<1$, where $M=2m_1+m_2$. The correctness of the present calculation is indicated by the agreement between our ϵ at $m_2/M\approx 1$ and the value for H^- calculated by Bhatia[3] (see Table I). Bhatia's dissociation energy is better than the one calculated here because he used more terms (90 instead of 70) and he used a different and presumably more optimal value of $\alpha/\beta=0.32$. The present choice of $\alpha/\beta=\frac{1}{4}$ is a compromise between Bhatia's α/β which works well for H^- and a very small α/β which for a given Ω would give smaller positive values of ϵ in the forbidden region near $m_2/M=\frac{1}{2}$. Near the extremes at $m_2/M=0$ or 1 the $^3P^e$ state is stable, but for $m_2\approx m_1$ it is not stable at our present level of approximation. Only negative values of ϵ represent a meaningful upper limit on the binding energies since $\epsilon=0$ representing a free particle plus an $n=2$ atom is obviously a lower-energy state than any $\epsilon>0$ configuration. The present results suggest that for $0.2<m_2/M<0.8$ and therefore for Ps^- the $^3P^e$ state does not exist. It might be interesting to do a calculation with a magnetic field included to see if any experimentally interesting binding energy for Ps^- would result for reasonable field strengths.

Since Fig. 1 shows that $^3P^e$ states are metastable for $0\leq m_2/M<0.175$ and $0.894<m_2/M<1$,[10] we now know that in addition to H^-, the following ions have a $^3P^e$ state: the muonium negative ion $\mu^+e^-e^-$, the hydrogen molecular ion H_2^+, and the muonic hydrogen molecular ion $p^+\mu^-p^+$. Our calculated values for the dissociation energies of these states are given in Table I. The $^1S^e$ (ground-state) dissociation energies are taken from the literature.[3,4,7,11]

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