Photodetachment of the positronium negative ion

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Recent interest in the properties of the negative ion of positronium has encouraged us to compute its cross section for photodetachment. To simplify the calculation, we have used the asymptotic form of the bound-state wave function and a plane wave for the final-state wave function, following the work of Ohmura and Ohmura in the case of photodetachment of H^-. We have obtained the needed normalization constant from a very precise and extensive Hylleraas wave function for the three-particle bound state.

The positronium negative ion (Ps^-) has for years[1] been known to be particle stable and has been the subject of many theoretical investigations,[2-4] but only recently has it been produced in the laboratory.[5] Further investigations have resulted in good measurements[6] of its annihilation lifetime, which agree within experimental uncertainty with theory.[3,4] It has also been suggested[5] that Ps^- could be used to generate positronium (Ps) beams of controlled energy; this would involve acceleration of Ps^- ions and photodetachment of one electron. For this application, as well as on general principles, it would be interesting to know the photodetachment cross section of Ps^-.

The formulation of the problem is straightforward: The dipole transition matrix element is calculated with use of a sufficiently accurate initial wave function of the bound ionic state as well as a p-wave continuum function describing the e^--Ps final state. In this report we will describe a calculation which simplifies the description of the initial bound state by representing it by an asymptotic form whose normalization comes from the most accurate Hylleraas wave function of the ion.[4] [This is justified by the very small binding energy (0.326 eV) of the Ps^- ion]. We make a further simplifying assumption by taking the final state to be a plane wave. (Note that some work designed to take into account the scattering has already been done.[7])

In Rydberg atomic units, the Hamiltonian of the system consisting of two electrons ($\boldsymbol{\rho}_1, \boldsymbol{\rho}_2$) and one positron ($\mathbf{x}$) is

$$H = -\nabla^2_{\boldsymbol{\rho}_1} - \nabla^2_{\boldsymbol{\rho}_2} - \nabla^2_{\mathbf{x}} - \frac{2}{|\boldsymbol{\rho}_1 - \mathbf{x}|} - \frac{2}{|\boldsymbol{\rho}_2 - \mathbf{x}|} + \frac{2}{|\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|} \ . \tag{1}$$

For the initial bound state of Ps^-, it is convenient to transform to the following center-of-mass coordinate system:

$$\mathbf{R} = \tfrac{1}{3}(\boldsymbol{\rho}_1 + \boldsymbol{\rho}_2 + \mathbf{x}), \quad \mathbf{r}_1 = \boldsymbol{\rho}_1 - \mathbf{x}, \quad \mathbf{r}_2 = \boldsymbol{\rho}_2 - \mathbf{x} \ , \tag{2}$$

where $\mathbf{R}$ is the coordinate of the center of mass of the entire system, and the other two coordinates measure the distances between the electrons and the positron. In these coordinates the Hamiltonian takes the following symmetric form:

$$H_s = -\tfrac{1}{3}\nabla^2_{\mathbf{R}} - 2\left[\nabla^2_{\mathbf{r}_1} + \nabla^2_{\mathbf{r}_2} + \nabla_{\mathbf{r}_1}\cdot\nabla_{\mathbf{r}_2} + \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}}\right] \ . \tag{3}$$

Omitting $\mathbf{R}$, which describes uniform motion of the center of mass, we previously wrote a wave function for the Ps^- ground state in the Hylleraas form as follows:

$$\Psi_i(r_1,r_2,r_{12}) = \sum_{l,m,n} C(l,m,n)\,[r_1^l r_2^m e^{-(\gamma r_1 + \delta r_2)} + r_2^l r_1^m e^{-(\gamma r_2 + \delta r_1)}] r_{12}^n \ , \tag{4}$$

and obtained an extremely accurate variational energy.[4] For the final state of the photodetachment, on the other hand, it is more appropriate to describe the $Ps + e^-$ system in an asymmetric form, since the correct kinematic description involves the motion of an electron relative to the center-of-mass of the Ps atom. That is, we use the coordinate $\mathbf{R}_2 = \mathbf{r}_2 - \mathbf{r}_1/2$ in place of $\mathbf{r}_2$, while retaining the other coordinates as before. The Hamiltonian in these unsymmetric coordinates is

$$H_u = -2\left[\nabla^2_{\mathbf{r}_1} + \tfrac{3}{4}\nabla^2_{\mathbf{R}_2} + \frac{1}{r_1} + \frac{1}{|\mathbf{R}_2 + \frac{1}{2}\mathbf{r}_1|} - \frac{1}{|\mathbf{R}_2 - \frac{1}{2}\mathbf{r}_1|}\right] \ . \tag{5}$$

The final state, involving the relative motion of a free electron and Ps in the ground state, must be a p state. In this paper, we will assume that the scattering in the p state is very small, and will write the final-state wave function as a properly symmetrized product of the Ps wave function and (the p-wave part of) a plane wave in the relative coordinate:

$$\Psi_f = \frac{1}{\sqrt{2}}[\phi(r_1)e^{i\mathbf{k}\cdot\mathbf{R}_2} + \phi(r_2)e^{i\mathbf{k}\cdot\mathbf{R}_1}], \quad \text{where } E = \tfrac{3}{2}k^2 \ . \tag{6}$$

Given the above forms for the initial and final wave functions, the photodetachment cross section can be written as[8]

$$\sigma_V = \frac{2k\alpha a_0^2}{9\omega}\,|\langle\Psi_f|Q_V|\Psi_i\rangle|^2 \ , \tag{7}$$

where the dipole transition operator in the velocity form is

$$Q_V = 2\hat{\mathbf{k}}\cdot(\nabla_{\boldsymbol{\rho}_1} + \nabla_{\boldsymbol{\rho}_2} - \nabla_{\mathbf{x}}) \ , \tag{8}$$

in terms of the fine-structure constant α, the unit wave vector of the relative Ps-e^- motion $\hat{\mathbf{k}}$, and the energy of the incident light ω. [In Eq. (7) the effect of the relationship between energy and relative momentum in the final state has been taken into account; it gives a factor of $\frac{2}{3}$ when compared with photodetachment from an infinitely massive

atomic ion.] In the usual way[8] the cross section can be rewritten in the length form

$$\sigma_L = \tfrac{2}{9} k\omega\alpha a_0^2 |\langle \Psi_f | Q_L | \Psi_i \rangle|^2 \ , \tag{9}$$

where the dipole transition operator in the length form is

$$Q_L = \hat{\mathbf{k}} \cdot (\boldsymbol{\rho}_1 + \boldsymbol{\rho}_2 - \mathbf{x}) \ . \tag{10}$$

These transition operators can be rewritten in terms of the unsymmetric relative coordinates:

$$\begin{aligned} Q_V &= \hat{\mathbf{k}} \cdot (\tfrac{2}{3}\nabla_R + 4\nabla_{r_1} + 2\nabla_{R_2}) \ , \\ Q_L &= \hat{\mathbf{k}} \cdot (\mathbf{R} + \mathbf{r}_1 + \tfrac{2}{3}\mathbf{R}_2) \ . \end{aligned} \tag{11}$$

So far, the only approximation made has been the use of plane waves in the final state [Eq. (6)]. At this point we make the second simplifying assumption; we represent the initial bound state in the following asymptotic form:

$$\Psi_i = C \frac{e^{-\gamma R_j}}{R_j} \phi(r_k), \quad \text{for } R_j >> r_k \ . \tag{12}$$

This approximation was first introduced, for deuteron photodissociation, by Bethe,[9] and its justification was the fact that the weakly bound deuteron is almost always outside the range of the forces, where the asymptotic form is quite accurate, especially for lower energies which do not probe the inner parts of the system in detail. Since then, it has been used many times, mainly for the similarly weakly bound ground state of H^-, for photodetachment,[10] and also for calculations of polarizability and other matrix elements.[11] [This approximation is even more useful for Ps^- than for H^-. Without it one would need to evaluate expressions containing mixed coordinates: r_1, r_2, r_{12} from Eq. (4), as well as R_j from Eq. (6).] Since the electron affinity of Ps is only about half that of H, we expect the approximation to be good in the present application also. The constant C is either the normalization constant of the asymptotic wave function taken literally (the zero-range approximation), or, better, it is obtained from a detailed wave function like our Eq. (4).

Inserting the appropriate constants and dropping the operators not involving R_2, which do not contribute to the photodetachment process in this approximation, we finally obtain

$$\begin{aligned} \sigma_V &= (3.0274 \times 10^{-20}\ \text{cm}^2) \frac{k}{(\gamma^2 + k^2)} |M_V|^2 \ , \\ \sigma_L &= (6.8115 \times 10^{-20}\ \text{cm}^2) k (\gamma^2 + k^2) |M_L|^2 \ , \end{aligned} \tag{13}$$

where we have set the Ps^- electron affinity equal to $3\gamma^2/2$. The two forms of the matrix element are written as follows:

$$\begin{aligned} M_V &= 2\sqrt{2}\, C \int d\mathbf{R} \frac{e^{-\gamma R}}{R} \hat{\mathbf{k}} \cdot \nabla_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \ , \\ M_L &= \frac{2\sqrt{2}}{3} C \int d\mathbf{R} \frac{e^{-\gamma R}}{R} \hat{\mathbf{k}} \cdot \mathbf{R} e^{i\mathbf{k}\cdot\mathbf{R}} \ . \end{aligned} \tag{14}$$

Since both the initial and final wave functions used here are eigenfunctions of a single local effective Hamiltonian, the usual derivation of the identity of the length and velocity forms of the cross section is valid; it is a useful check on our procedure that we do get the same result. That is,

$$\sigma_V = \sigma_L = (3.8245 \times 10^{-17}\ \text{cm}^2) \frac{k^3 C^2}{(k^2 + \gamma^2)^3} \ . \tag{15}$$

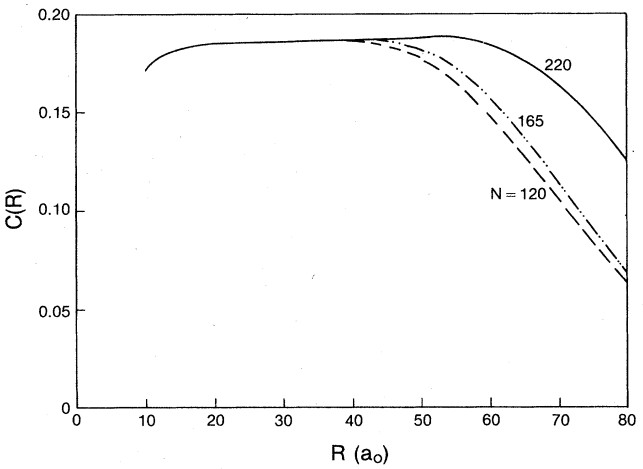

FIG. 1. Normalization constant $C(R)$, obtained from the Hylleraas wave function, as a function of the coordinate R. Note that the main effect of increasing the expansion length is to lengthen the plateau.

It remains to evaluate the constant C from the variational wave function[4] of Eq. (4). After setting $r_1 = 0$, $r_2 = r_{12} = R_2 = r$, we define $C(r)$ as

$$C(r) \equiv (8\pi)^{1/2} r e^{\gamma r} \Psi_i(0, r, r) \ , \tag{16}$$

where the numerical factor comes from the normalization of the Ps ground-state wave function ϕ. In Fig. 1 we have plotted $C(r)$ over a wide range in the "asymptotic" region to demonstrate its near constancy; from the plateau in the region $20 < R < 40$ we obtain the value $C = 0.1856(2)$. Our final result for the photodetachment cross section is, in terms of the relative momentum k,

$$\sigma = (1.32 \times 10^{-18}\ \text{cm}^2) \frac{k^3}{(k^2 + \gamma^2)^3} \ , \tag{17}$$

or, in terms of the wavelength λ of the incident light,

$$\sigma = (650 \times 10^{-18}\ \text{cm}^2) \left(\frac{\lambda}{\lambda_0}\right)^{3/2} \left[1 - \frac{\lambda}{\lambda_0}\right]^{3/2}, \quad \text{for } \lambda \leq \lambda_0 \ . \tag{18}$$

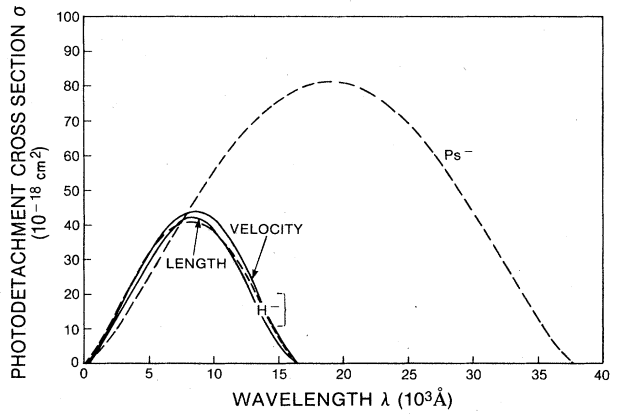

FIG. 2. Photodetachment cross sections (dashed lines) in the asymptotic approximation for Ps^- and H^- as functions of the wavelength of the incident light. The length and velocity forms of the H^- cross section are from the more elaborate theory of Ref. 12 (solid lines).

From Ref. 4 the best variational value of the Ps^- binding energy is 0.024 010 113 Ry, corresponding to $\gamma = 0.126\,517\,75$ and to a threshold wavelength $\lambda_0 = 379\,53.46$ Å. In Fig. 2 we have plotted the present results [Eq. (18)], compared with the corresponding results[10] for H^-. In the latter case the asymptotic approximation is seen to compare fairly well with the more elaborate calculations,[12] and we expect the present results to be similarly reliable.

One additional test of the calculation can be made. The result can be compared to the sum rule[12]

$$S_{-1} = \frac{1}{2\pi^2 \alpha a_0^2} \int_0^{\lambda_0} d\lambda \frac{\sigma}{\lambda}$$

$$= \tfrac{8}{27} \langle (\mathbf{r}_1 + \mathbf{r}_2)^2 \rangle = \tfrac{8}{27} [4\langle r_1^2 \rangle - \langle r_{12}^2 \rangle] , \qquad (19)$$

where the brackets represent expectation values in the Ps^- ground state. We obtain the values[13] $\langle r_1^2 \rangle = 48.4152$ and $\langle r_{12}^2 \rangle = 93.1714$; the left-hand side of Eq. (19) in the present approximation is 31.7, and the right-hand side is 29.775. Our approximate cross section thus exceeds the sum-rule limit by 6.5%, almost exactly the same error as in the case of H^-. Remember, however, that this sum rule emphasizes short wavelengths, where the approximation is poorest. Further work, involving better scattering functions, is to be encouraged.

Note added in proof. From the quantities γ and C it is possible to estimate the singlet e^--Ps scattering parameters at low energies [T. Ohmura, Y. Hara, and T. Yamanouchi, Prog. Theor. Phys. **20**, 82 (1958)]. The scattering length a and effective range r_0 (in units of a_0) satisfy the equations $r_0 = (1/\gamma) - (1/4\pi C^2)$, $(1/a) = \gamma - \frac{1}{2} r_0 \gamma^2$, from which we obtain the values $a = 12.233 \pm 0.006$ and $r_0 = 5.594 \pm 0.005$. The former agrees fairly well with the value $a = 12.38 \pm 0.07$ obtained by a direct Kohn variational calculation.[7]

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