THE PHOTODETACHMENT OF Ps^- and LOW-ENERGY e^+-H COLLISIONS

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ABSTRACT

Two calculations in the area of positron collisions are presented. The first is the calculation of the photodetachment cross section of the positronium negative ion (Ps^-) using accurate variational wave functions for both the initial bound-state and the final ^1P continuum state. The second is the calculation of partial wave cross sections for Ps($1s$)-formation in e^+-H($1s$) collisions using the hyperspherical hidden crossing method. Since the S-wave Stückelberg phase is close to π, the very small S-wave Ps($1s$) formation cross section can be understood in terms of destructive interference. Other examples in positron collisions are given where it is either known or expected that destructive interference is the cause of the small S-wave Ps($1s$) formation cross section. In addition, examples are presented of processes in atomic physics where the Stückelberg phase is a multiple of $\frac{\pi}{2}$.

I. INTRODUCTION

Dr. Richard Drachman has performed pioneering work in the theory of positron physics. He has been an encouragement and support to me since I was a graduate student. I appreciate Dr. Richard Drachman taking interest in my work and sharing his thoughts. In this paper, I describe some work I have performed with my collaborators on the photodetachment of the positronium negative ion Ps^- (section II) and on low-energy e^+-H($1s$) collisions (section III). These two problems have been of mutual interest to Dr. Richard Drachman and myself. Atomic units will be used in this paper unless explicitly stated.

II. PHOTODETACHMENT of Ps^-

The first interaction I remember with Dr. Richard Drachman was receiving his candid criticism, yet written in an encouraging way, of a preprint that Dr. M. R. C. McDowell (my Ph. D. supervisor) and I had written on e^--Ps when I was a beginning graduate student. As a student, I became interested in Bhatia and Drachman's pioneering calculation on the photodetachment of Ps^-. This calculation was performed shortly after the existence of Ps^- was experimentally verified [2]. Bhatia and Drachman employed the 'loosely' bound approximation which used the asymptotic form of an accurate initial bound-state wave function (220 linear parameters) and a plane-wave for the final-state wave function. They obtained an analytical expression for the photodetachment cross section,

$$a_\lambda(L,V) = (1.32 \times 10^{-18}\mathrm{cm}^2)\,\frac{k^3}{(k^2+\gamma^2)^3}\,, \qquad (1)$$

where k is the wave vector of the relative Ps-e^- motion. The term γ is defined in terms of the electron affinity of Ps^-, $\varepsilon_b = 3\gamma^2/4$. Since the initial and final wave functions are the eigenfunctions of the same model Hamiltonian, the length and velocity cross sections are identical. A similar calculation was performed by Ohmura and Ohmura [3] for H^- and has proven to be successful, especially at long wavelengths.

For my Ph.D., I studied e^--Ps scattering and the photodetachment of Ps^- for energies below the Ps($n = 2$) threshold. Humberston, McDowell and I [4] computed the photodetachment of Ps^-. We used an accurate variational wave function for the ground-state and obtained the ^1P continuum wave function for e^--Ps from the Kohn variational method. The ground-state wave function contained 95 linear parameters, whereas the ^1P continuum wave function contained 220 linear parameters. We computed the photodetachment cross section in both the length and velocity formulations.

Figure 1 shows Bhatia and Drachman's cross section with our length and velocity cross sections. The length and velocity cross sections are in excellent agreement with one another. Furthermore, Bhatia and Drachman's cross section agrees well with our cross sections for the overall shape and for the position of the maximum. However, the height of maximum in our cross sections is somewhat lower than in theirs.

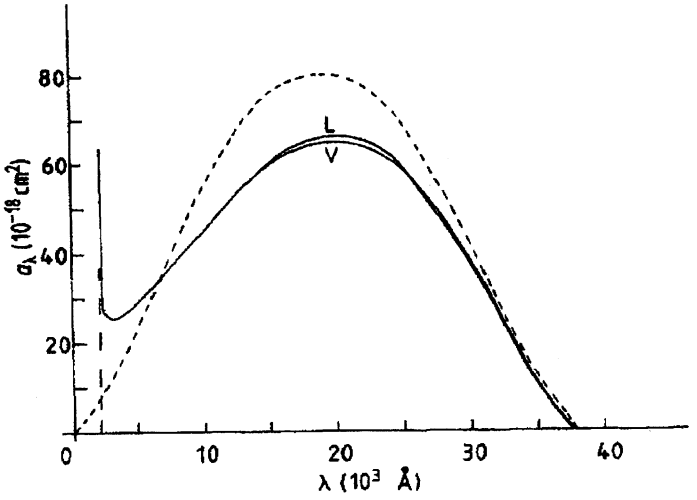

Figure 1. Photodetachment cross section of Ps^-. The L (V) marks the variational length (velocity) cross section. The dashed line (—) denotes Bhatia and Drachman's cross section. The vertical broken line indicates the position of the $n = 2$ threshold.

We followed Bhatia and Drachman in seeing how well the photodetachment cross section satisfies the sum rule

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

$$= \frac{8}{27} \left\langle \Psi_i \middle| |\mathbf{r}_1 + \mathbf{r}_2|^2 \middle| \Psi_i \right\rangle , \tag{2b}$$

where λ_0 is the threshold wavelength and Ψ_i is the initial-state wave function of Ps^-. In

our variational calculations, we had considered energies only up to the $n = 2$ threshold. In evaluating S_{-1}, we used Bhatia and Drachman's analytical expression for a_λ for energies above the $n = 2$ threshold. The contribution to S_{-1} for these energies is small.

In Table 1 we compare Eq. (2a) with Eq. (2b) evaluated using the length (WHML) and the velocity (WHMV) formulation of the photodetachment cross section. We compare our evaluation of S_{-1} with that evaluated by Bhatia and Drachman, in which they used their 220 linear parameter wave function Ψ_i in Eq. (2b). The velocity results show a discrepancy of less than 2%, the length results show a discrepancy of less than 1%, while Bhatia and Drachman's results show a discrepancy of -6.5%. Thus, by comparing Bhatia and Drachman's photodetachment cross section and the sum rule S_{-1} with the results obtained with the elaborate variational wave functions, it can be seen that the 'loosely' bound approximation works well for Ps^-. This is what Bhatia and Drachman [1] had expected in light of the very small binding energy of Ps^- and the comparison for H^- of the photodetachment cross section computed with the same approximation with an elaborate calculation [8].

Table 1. Values of the sum Rule S_{-1}

Source	(2a)	(2b)
WHML [4]	29.5	29.75
WHMV [4]	29.2	29.75
Bhatia and Drachman [1]	31.7	29.775

To test the accuracy of our 95 linear parameter initial-state wave function of Ps^-, we computed the electron affinity of Ps^- and obtained a value of 0.012004615 [5]. The most accurate prediction of the electron affinity at the time of our calculation was the calculation performed by Bhatia and Drachman [6] using their 220 linear parameter Hylleraas wave function. They obtained the value of 0.012005057 [6]. Using the Kohn variational method, we also computed the singlet and triplet S- and P-wave scattering phase shifts for e^--Ps scattering for energies below the Ps($n = 2$) threshold [4,7]. From S-wave phase shifts we obtained a value of 12.0 ± 0.3 for the singlet S-wave scattering length and a value of 4.6 ± 0.4 for the triplet [4]. From their 220 linear parameter Ps^- bound state wave function, Bhatia and Drachman [9] deduced a value for the singlet S-wave scattering length of 12.233 ± 0.006. The two sets of singlet S-wave scattering lengths agree to within the error bars.

III. e^+-H COLLISIONS

The problem of e^+-H collisions is of interest in astrophysics due to the observation of 511-keV line γ rays from solar flares, the galactic center and above the galactic center [10-12]. Analysis of the width of the 511-keV line using accurate Ps formation cross sections for e^+-H collisions provides information on the ionization state and temperature of the radiating medium. Dr. Richard Drachman studied e^+-H collisions over 30 years ago. For instance, he and his collaborators performed a rigorous bound-state calculation of e^+-H collisions for energies below the Ps formation threshold [13]. They used a generalized Hylleraas function which explicitly included a virtual Ps factor and computed the S-wave phase shifts for e^+-

H($1s$) collisions. In addition to this calculation, Houston and Drachman [14] computed S-wave phase shifts for e^+-H($1s$) collisions below the Ps($1s$) formation threshold using the Harris variational method and scattering lengths using the Kohn variational method. These variational calculations are still considered today as benchmark calculations [15].

Fairly recently, Macek, Ovchinnikov and I applied the hyperspherical hidden crossing method (HHCM) to Ps($1s$) formation in e^+-H($1s$) collisions for energies within the Ore gap [16]. This method had been formulated by Macek and Ovchinnikov to treat the correlated motion of three charged particles of arbitrary mass and charge [17]. The most attractive feature of the HHCM is that it provides insight into the scattering processes. Furthermore, it is ideally suited to treat rearrangement collisions since it treats the rearrangement and excitation on an equal footing.

For the case where there are only two open channels, the S-matrix modulus squared term $|\tilde{S}_{ij}|^2$ for the transition between two levels i and j is given by

$$|\tilde{S}^L_{ij}|^2 = 4P^L_{ij}(1 - P^L_{ij}) \sin^2 \Delta^L_{ij}, \tag{3}$$

where the Stückelberg phase Δ^L_{ij} is

$$\Delta^L_{ij} = \Re \int_C K(R) dR \tag{4}$$

and the one-way transition probability P^L_{ij} is

$$P^L_{ij} = \exp\left(- 2 \Im \int_C K(R) dR \right). \tag{5}$$

The wave vector in the HHCM is defined in terms of the adiabatic energy eigenvalues ε_μ

$$K^2_\mu(R) = 2\left(E - \varepsilon_\mu(R) - \frac{1}{8R^2} \right), \tag{6}$$

where E is the total energy of the three particle system. The contour integral C in Eqs.(4) and (5) starts at the classical turning point R^t_i of $\varepsilon_i(R)$, goes clockwise around the branch point R_b that connects levels i and j, and ends at the classical turning point R^t_j of $\varepsilon_j(R)$.

We computed the S-, P-, and D-wave cross section for Ps($1s$) formation in e^+-H($1s$) collisions in the Ore gap [16]. The P- and D-wave results compared reasonably well with the Kohn variational [18-19] and the Harris-Nesbet [20] results benchmark calculations, respectively. As showed by Humberston [21-22] using the Kohn variational method, the S-wave cross section is very small, except very close to the threshold. The reason for this can be understood from the HHCM [16]. The S-wave Stückelberg phase is close to π, which means that the two amplitudes corresponding to different paths leading to Ps formation destructively interfere. The D-wave contribution to the Ps formation cross section is dominant for about two-thirds of the energy range [16,19,20]. The D-wave Stückelberg phase is close to $\frac{\pi}{2}$, so that there is constructive interference between the two amplitudes that correspond to different paths leading to Ps formation.

Recently, using the HHCM, Shertzer and I [23] computed the S-, P-, D- and F-wave cross section for Ps($1s$) formation in e^+-Li($2s$) collisions in the energy range 0-1.8 eV. In this

energy range, there are only two open channels, elastic scattering and Ps(1s) formation. We confirmed the conclusion of Kohn variational results [24], namely, that away from threshold the S-wave cross section for Ps($1s$) formation in e^+-Li($2s$) collisions is very small. As for e^+-H($1s$), the S-wave Stückelberg phase is close to π, so that there occurs destructive interference between the two amplitudes corresponding to different paths leading to Ps($1s$) formation. At a particular energy, the Stückelberg phase is exactly π which gives a minimum in the Ps($1s$) formation cross section.

Using the Kohn variational method, Van Reeth and Humberston [25] computed the S-, P- and D-wave cross sections for Ps($1s$)-formation in e^+-He collisions in the Ore gap. They found the S-wave Ps($1s$) formation cross section is very small. It may be a universal result that the $L = 0$ Ps($1s$) formation cross section for e^+ collisions with any atom in a S ground-state is small. If so, our HHCM studies of e^+-H($1s$) [16] and e^+-Li($2s$) collisions [23] would suggest that the reason is due to destructive interference and that the Stückelberg phase is close to a multiple of π. Interestingly, McAlinden et. al. [26] recently noted for e^+-H^- collisions at 0.1eV, the S-wave contribution to Ps($1s$) formation cross section is small and the D-wave is dominant. The e^+-H^- collisions problem has been of interest to Dr. Richard Drachman. Straton and Drachman [27] applied orthogonalization corrections to the Coulomb (1^{st} order) Born approximation (CBA) to compute differential and total cross sections for Ps($1s$) formation in e^+-H^- collisions.

The reason why the Stückelberg phase should be close to π for S-wave Ps($1s$) formation in e^+-H($1s$) and e^+-Li($2s$) collisions is not known. There are, however, other examples in the literature of the Stückelberg phase being an integer values of $\frac{\pi}{2}$ which may help shed light on the reason. For instance, Ostrovsky [28] reported for the rearrangement process $d\mu(n_i) + t \rightarrow d + t\mu(n_f)$ for $L = 0$ Stückelberg phases close to integer multiples of $\frac{\pi}{2}$. In particular, for the $1s$-$1s$ transition, the Stückelberg phase is approximately 2π which means that reaction probability is strongly suppressed. This calculation [28] and our HHCM calculations [16,23] suggest that the Stückelberg phase is close to a multiple of π for a rearrangement process for a S ground-state to S ground-state transition. Nielsen and Macek [29] obtained a Stückelberg phase of 3π at a particular energy for the reaction $^4He + {}^4He + {}^4He \rightarrow {}^4He + {}^4He_2$ which gave a minimum in the S-wave transition probability. Miyashita et. al. [30] obtained a minimum in the transition probability for $L = 0$ electron-impact ionization of the collinear $Z = 1/4$ model atom. At the minimum the Stückelberg phase is a multiple of π.

Support from NSF, under grant PHY-0440565, is appreciated. Permission from IOP to reproduce the photodetachment, the sum rule and scattering length results from Ref. [4] is appreciated.

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