Positronium formation from H^-

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Positronium formation by electron capture from a negative hydrogen ion is studied with use of the Coulomb-Born approximation. Differential and integral cross sections are calculated by using the prior and the post form of the approximation for incident positron energy varying between 20 and 500 eV.

I. INTRODUCTION

Recently Drachman[1] has discussed the importance of the process of positronium (Ps) formation in collisions between positrons and negative hydrogen ions (H^-). Since the electron affinity of H is less than the binding energy of the first few states of positronium, Ps formation in these states can take place even at zero energy and the process may be of interest in the transition zone of planetary nebulas.

The formation of positronium in e^+-atom scattering is a rearrangement transition and the first theoretical study was made by Massey and Mohr,[2] who applied the method of first Born approximation (FBA) for an atomic hydrogen (H) target. Since then, the second Born and the Padé approximation,[3] the variational method,[4] the hybrid approximation,[5] and a number of other methods[6] have been used (mainly for H and He targets) depending upon the energy of the incident positron. Experimental measurement of the cross section for positronium formation has also been made for some gases and the progress achieved has been reviewed by Griffith.[7] At present it does not seem possible to have a laboratory measurement of positronium formation in negative hydrogen ions. Any theoretical calculation for the process must take proper care of the long-range Coulomb interaction between the positron and H^-, and this makes the application of many of the methods mentioned above rather complicated. As the Coulomb-Born approximation (CBA) (Ref. 8) is a simple method which ensures a correct handling of the residual Coulomb interaction between the collision partners at large distance, we have, in the present work, used it to determine the cross section for Ps formation in the ground state in e^+-H^- collisions. The hydrogen atom that is left after electron transfer is assumed to remain in its ground state. The calculation has been done for incident positron energy ranging between 20 and 500 eV. The CBA is not expected to be a good approximation at low incident energy but, in the absence of any other more accurate calculation, we have used it down to 20 eV.

The theory of the method is given in Sec. II of the paper. The results are presented and discussed in Sec. III. Atomic units will be used throughout except for integral cross sections which will be expressed in πa_0^2.

II. THEORY

The initial and final systems in the rearrangement transition

$$e^+ + H^- \rightarrow H(1s) + Ps(1s) \tag{1}$$

are shown in Fig. 1. The proton is considered to be at rest and the position vectors of the two electrons from it are $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. $\mathbf{R}_i$ represents the position vector of the positron with initial momentum $\mathbf{k}_i$, and $\mathbf{R}_f$ is the position vector of the center of mass of the positronium with final momentum $\mathbf{k}_f$. $\mathbf{r}_1'$ and $\mathbf{r}_2'$ will denote, respectively, the distances of the two electrons from the positron.

The rearrangement T-matrix element in the distorted-wave approximation may be written as[9,10]

$$T_{fi} = \langle \xi_f^- \mid V_i - U_i \mid \chi_i^+ \rangle \tag{2a}$$

or

$$T_{fi} = \langle \xi_f^- \mid V_f - U_f \mid \chi_i^+ \rangle \ , \tag{2b}$$

where

$$V_i = \frac{1}{R_i} - \frac{1}{r_1'} - \frac{1}{r_2'}$$

and

$$V_f = \frac{1}{R_i} - \frac{1}{r_1} - \frac{1}{r_2'} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \ .$$

U_i and U_f are suitable distorting potentials in the initial

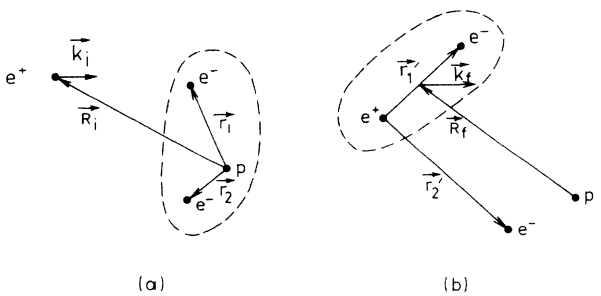

FIG. 1. The initial (a) and final (b) systems in the transition $e^+ + H^- \rightarrow H(1s) + Ps(1s)$.

and final channels, the corresponding distorted channel states with appropriate boundary conditions being χ_i^+ and ξ_f^-, respectively. In Eq. (2a) U_f may be chosen arbitrarily but U_i should be chosen such that χ_i^+ does not contain a component corresponding to a rearrangement from the initial channel. In Eq. (2b), on the other hand, U_i is arbitrary but U_f should be such that ξ_f^- contains no component corresponding to a rearrangement from the final channel.

If in Eq. (2a) we take $U_f=0$ and $U_i=-1/R_i$, so that in coordinate representation

$$\xi_f^- = \phi_{\rm Ps}(\mathbf{r}_1')\phi_{\rm H}(\mathbf{r}_2)\exp(i\mathbf{k}_f\cdot\mathbf{R}_f) \tag{3}$$

and

$$\chi_i^+ = \phi_{\rm H^-}(\mathbf{r}_1,\mathbf{r}_2)\chi_c^+(\mathbf{k}_i,\mathbf{R}_i)\ , \tag{4}$$

where $\phi_{\rm Ps}$, $\phi_{\rm H}$, and $\phi_{\rm H^-}$ are the ground-state wave functions of the positronium, the hydrogen atom, and the negative hydrogen ion, respectively, and $\chi_c^+(\mathbf{k}_i,\mathbf{R}_i)$ is the Coulomb wave function

$$\chi_c^+(\mathbf{k}_i,\mathbf{R}_i) = \exp(i\mathbf{k}_i\cdot\mathbf{R}_i)\exp(-\tfrac{1}{2}\pi\nu_i)\Gamma(1+i\nu_i) \times F(-i\nu_i,1,i(k_iR_i-\mathbf{k}_i\cdot\mathbf{R}_i)) \tag{5}$$

with

$$\nu_i = -1/k_i\ ,$$

then the transition matrix element becomes

$$T_{fi}^{\rm prior} = \int\int\int \phi_{\rm Ps}^*(\mathbf{r}_1')\phi_{\rm H}^*(\mathbf{r}_2)\exp(-i\mathbf{k}_f\cdot\mathbf{R}_f) \times\left(\frac{2}{R_i}-\frac{1}{r_1'}-\frac{1}{r_2'}\right) \times\phi_{\rm H^-}(\mathbf{r}_1,\mathbf{r}_2)\chi_c^+(\mathbf{k}_i,\mathbf{R}_i)d\mathbf{R}_i\,d\mathbf{r}_1\,d\mathbf{r}_2\ . \tag{6a}$$

This is what is known as the CBA in its prior form.

Alternatively, we can make the same choice of U_i and U_f in Eq. (2b) to get the transition matrix element in the post form of the CBA,

$$T_{fi}^{\rm post} = \int\int\int \phi_{\rm Ps}^*(\mathbf{r}_1')\phi_{\rm H}^*(\mathbf{r}_2)\exp(-i\mathbf{k}_f\cdot\mathbf{R}_f) \times\left(\frac{1}{R_i}-\frac{1}{r_1}-\frac{1}{r_2'}+\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\right) \times\phi_{\rm H^-}(\mathbf{r}_1,\mathbf{r}_2)\chi_c^+(\mathbf{k}_i,\mathbf{R}_i)d\mathbf{R}_i\,d\mathbf{r}_1\,d\mathbf{r}_2\ . \tag{6b}$$

Remembering that any one of the electrons may be cap-

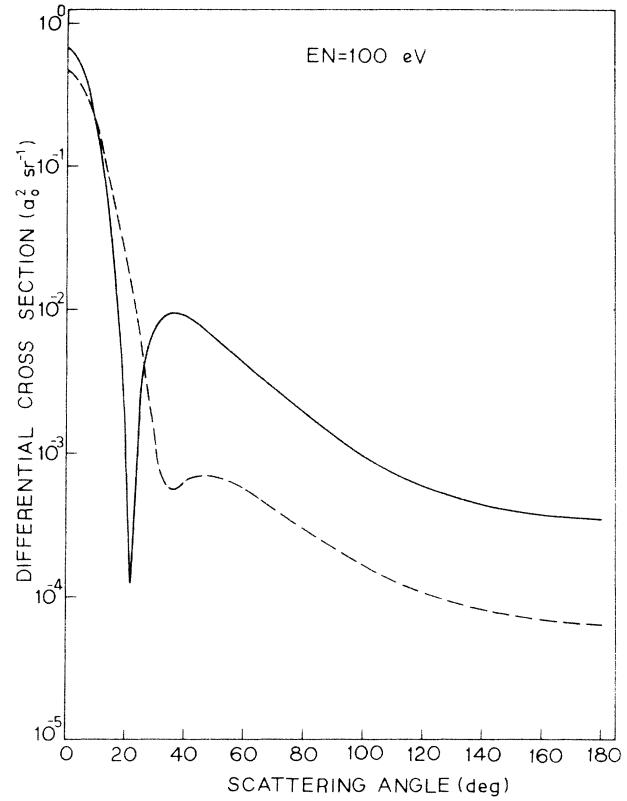

FIG. 2. Differential cross sections for positronium formation in the ground state by electron capture from a negative hydrogen ion for an incident positron energy of 100 eV. ——, prior interaction; — — —, post interaction.

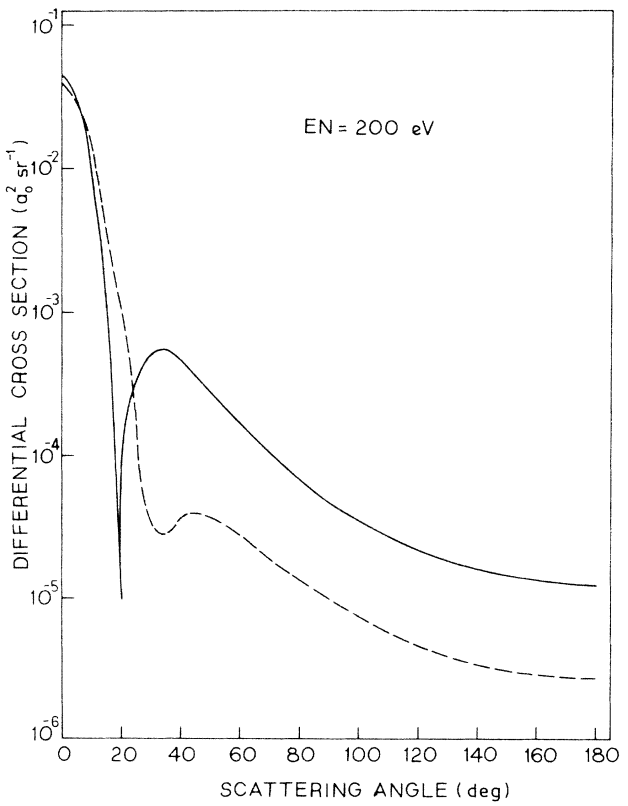

FIG. 3. Differential cross sections for positronium formation in the ground state by electron capture from a negative hydrogen ion for an incident positron energy of 200 eV. ——, prior interaction; — — —, post interaction.

tured by the positron to form positronium, the differential scattering cross section for the process (1) is given by

$$I(\theta,\varphi)=\frac{1}{\pi^2}\frac{k_f}{k_i}|T_{fi}|^2 , \tag{7}$$

where the prior or the post form of T_{fi} may be used. The integral cross sections in the two approximations can now be obtained by integration over the angular variables.

We have employed the ground-state wave function of H^- given by Lowdin,[11]

$$\phi_{H^-}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{4\pi}[A\exp(-\alpha r_1)+B\exp(-\beta r_1)] \times[A\exp(-\alpha r_2)+B\exp(-\beta r_2)] . \tag{8}$$

The values of the parameters, A, B, α, and β are taken from the work just mentioned. The hydrogen and positronium wave functions are of the standard form

$$\phi_H(\mathbf{r}_2)=\left[\frac{\lambda^3}{\pi}\right]^{1/2}\exp(-\lambda r_2),\quad \lambda=1.0 , \tag{9}$$

and

$$\phi_{Ps}(\mathbf{r}_1')=\left[\frac{\mu^3}{\pi}\right]^{1/2}\exp(-\mu r_1'),\quad \mu=0.5 . \tag{10}$$

In order to evaluate T_{fi}^{prior} given by Eq. (6a) we have first changed the integration variables to $\mathbf{R}_i$, $\mathbf{r}_1'$, and $\mathbf{r}_2$. The integration over $\mathbf{r}_2$ is straightforward and that over $\mathbf{r}_1'$ is reduced to one-dimensional integration by using Fourier transforms and Feynman parametrization technique. We have then

$$T_{fi}^{\text{prior}}=\int J(\mathbf{k}_f,\mathbf{R}_i)\exp(-i\mathbf{k}_f\cdot\mathbf{R}_i)\chi_c^+(\mathbf{k}_i,\mathbf{R}_i)d\mathbf{R}_i , \tag{11}$$

where

$$J(\mathbf{k}_f,\mathbf{R}_i)=-4(\mu\lambda)^{3/2}\left[\left[\frac{A}{(\lambda+\alpha)^3}+\frac{B}{(\lambda+\beta)^3}\right]+[Af(\lambda+\alpha,R_i)+Bf(\lambda+\beta,R_i)]\frac{\partial}{\partial\mu}\right] \times\int_0^1 dx\exp[i\tfrac{1}{2}\mathbf{k}_f\cdot\mathbf{R}_i(1-x)]\left[A\alpha x\left[\frac{1}{L^3(x)}+\frac{R_i}{L^2(x)}\right]\exp[-R_iL(x)] +B\beta x\left[\frac{1}{M^3(x)}+\frac{R_i}{M^2(x)}\right]\exp[-R_iM(x)]\right] , \tag{12}$$

with

$$f(\nu,R_i)=\frac{1}{\nu^3}\left[\frac{1}{R_i}+\left[\frac{1}{R_i}+\frac{\nu}{2}\right]\exp(-\nu R_i)\right] , \tag{13}$$

$$L^2(x)=\alpha^2x+\mu^2(1-x)+\tfrac{1}{4}k_f^2x(1-x) , \tag{14}$$

and

$$M^2(x)=\beta^2x+\mu^2(1-x)+\tfrac{1}{4}k_f^2x(1-x) . \tag{15}$$

Noting the expression (5) for the Coulomb wave function and the result[12]

$$\int\frac{1}{R_i}\exp(-LR_i+i\mathbf{t}\cdot\mathbf{R}_i)F(-i\nu_i,1,i(k_iR_i-\mathbf{k}_i\cdot\mathbf{R}_i))d\mathbf{R}_i =4\pi\frac{(L^2+t^2)^{-i\nu_i-1}}{[L^2+t^2-2(iLk_i+\mathbf{t}\cdot\mathbf{k}_i)]^{-i\nu_i}} , \tag{16}$$

T_{fi}^{prior} may be expressed as an integral over x from 0 to 1 with a rather lengthy integrand whose expression is not given here. The integral over x is evaluated for each set of values of incident energy and angle of scattering by using a Gaussian quadrature formula with a sufficient number of quadrature points to ensure convergence. The differential cross sections for positronium formation in H^- are then obtained using Eq. (7). The integral cross sections in CBA (prior) are evaluated by another numerical integration.

An analogous technique has been used to determine the

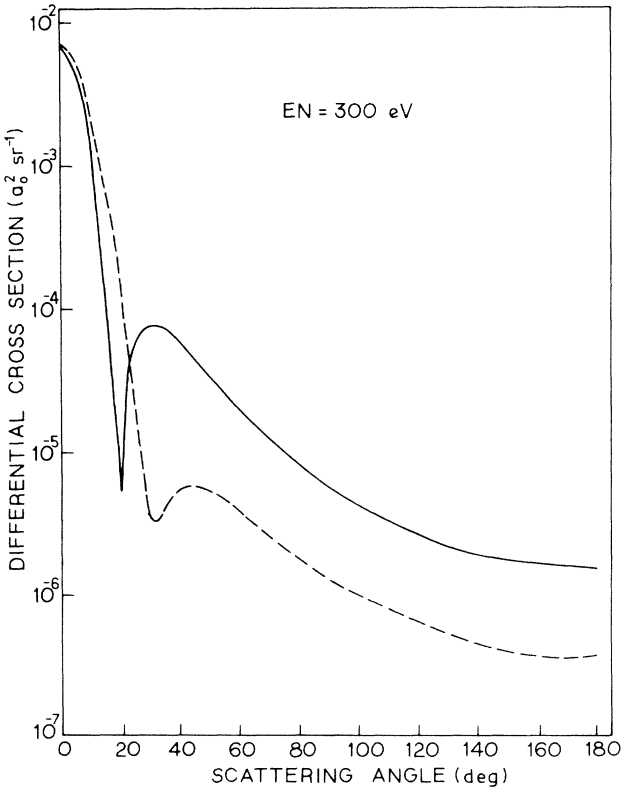

FIG. 4. Differential cross sections for positronium formation in the ground state by electron capture from a negative hydrogen ion for an incident positron energy of 300 eV. ——, prior interaction; — — —, post interaction.

TABLE I. Integral cross sections for positronium formation in the ground state by electron capture from a negative hydrogen ion. (Figures within parentheses indicate the powers of ten by which the numbers are to be multiplied.)

Incident energy (eV)	Integral cross section in πa_0^2 Prior	Post
20	0.348(1)	0.153(1)
50	0.294(0)	0.161(0)
100	0.255(−1)	0.179(−1)
200	0.129(−2)	0.125(−2)
300	0.181(−3)	0.213(−3)
500	0.127(−4)	0.187(−4)

cross sections in the post form of the CBA. This time, however, we have found it convenient to start with the integration variables $\mathbf{R}_i$, $\mathbf{r}_1$, and $\mathbf{r}_2$ as given in Eq. (6b).

III. RESULTS AND DISCUSSION

We present in Table I our results for integral cross sections for positronium formation in the ground state by electron capture from H^-. The cross sections have been determined for both the prior and the post forms of the CBA for incident positron energy varying between 20 and 500 eV. The difference between the "prior" and the "post" cross sections indicates the approximate nature of the wave function [Eq. (8)] for the negative hydrogen ion. For other two-electron atoms or ions, cross sections for electron capture are often calculated using a one-parameter wave function of the Hylleraas form.[13] But we see that, for H^-, even with a three-parameter wave function, a considerable amount of post-prior discrepancy remains. This is presumably due to the loose structure of the negative hydrogen ion.

The differential cross sections for the process (1) at 100, 200, and 300 eV are shown graphically in Figs. 2–4. Each of the figures contains the results obtained with the prior and post interactions. Every curve shows the occurrence of a minimum at some angle of scattering. These are due to cancellation in part of the contributions coming from the interaction between oppositely charged particles by those coming from the interaction between like charges. The position of the minimum depends upon the energy of the incident positron—it shifts towards lower scattering angle with increase in incident energy.

Since there are no other theoretical or experimental results available for the cross section for positronium formation in H^-, it is not possible to make any definite conclusion regarding the range of incident positron energy for which the CBA will have sufficient accuracy. However, the method is simple enough to give a quick estimate of the rate of this important process and can be easily adapted to study the effect of the use of a more complicated wave function of H^-.

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