Evaluation of cross section for electron capture by positrons

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We present an improved method for the calculation of positronium-formation cross section from one-electron atomic targets of arbitrary charge Z_T. The calculation is complete through second order in the collisional potentials. We use this technique to calculate the positronium-formation cross sections for 1s-1s electron capture from atomic hydrogen.

I. INTRODUCTION

With positrons it is now possible to achieve an understanding of high-velocity rearrangement collision that is not possible with heavier projectiles. Because the positron is of identical mass and opposite charge to the electron, observable interference effects can occur with positrons but not with protons. Moreover, positronium (Ps) formation in a bound electron-antielectron state is an interesting phenomenon in total positron-atom scattering events, which sets it apart from electron-atom scattering where capture is not possible. The conceptually important Thomas peak is a prominent feature in the differential cross section well established by various measurements[1,2] and calculations[3-10] for electron capture by heavier projectiles. But for electron capture by positrons the Thomas peak is expected to vanish due to the dynamical interference first noted by Shakeshaft and Wadehra[11] (hereafter called SW), who presented a method for calculation of positronium-formation cross section in the distorted-wave Born approximation. However, SW used plane-wave intermediate states, which are not always adequate to describe the angular distribution near the Thomas peak as pointed out by Briggs *et al.*[6] Since new experimental data[12,13] for the Ps formation are now rapidly accumulating, the need for a better theoretical method is now evident.

In Sec. II we present a method for the calculation of Ps-formation cross section from a one-electron atom. Our calculation is the first calculation correct through all second-Born terms. The present method differs from the strong potential Born (SPB) approximation in two ways. First, our method includes the internuclear potential excluded in SPB. Second, we include a second-order distortion term not present in SPB. Furthermore, we have used the positronium intermediate states in our dominant amplitude instead of the simpler plane-wave intermediate states used by Shakeshaft and Wadehra.[11]

The present technique is based in part on the technique of Sil and McGuire[10] (hereafter called SM). Out of the four second-order terms in our calculations we evaluate the two dominant terms following SM, but using a different Green's function. SM used the target Green's function which includes the electron-target potential to all orders, whereas we use the projectile Green's function that includes positron-electron interaction to all orders. The two other second-order terms, called second-order distortion terms, have not been previously considered. The total transition matrix element is finally reduced to a one-dimensional integral which is to be evaluated numerically. Our recent calculation[14] is based on the leading-order terms of this calculation.

II. THEORY

Let a fast positron capture an electron from a target atom of effective nuclear charge Z_T. The coordinate system is shown in Fig. 1 and atomic units will be used throughout the calculation. The full Hamiltonian for the positron-atom system (we consider here only the active electron, target nucleus, and the positron in this system) can be written as

$$H = H_i + \bar{V}_i \tag{1a}$$

or as

$$H = H_f + \bar{V}_f \; , \tag{1b}$$

where

$$\begin{aligned} H_i &= -\tfrac{1}{2}\nabla_r^2 - \tfrac{1}{2}\nabla_R^2 - \frac{Z_T}{r} \; , \\ H_f &= -\frac{1}{2\mu}\nabla_\rho^2 - \frac{1}{2M}\nabla_S^2 - \frac{1}{\rho'} \\ \bar{V}_i &= \frac{Z_T}{R} - \frac{1}{\rho}, \quad \bar{V}_f = \frac{Z_T}{R} - \frac{Z_T}{r}, \quad \mu = \tfrac{1}{2}, \quad M = 2 \; . \end{aligned} \tag{2}$$

The transition matrix element for electron capture by the positron from the target atom is then given by

$$T = \langle \psi_f \mid \bar{V}_f (1 + G^+ \bar{V}_i) \mid \psi_i \rangle \; , \tag{3}$$

where $G^+ = (E - H + i\eta)^{-1}$ and ψ_i and ψ_f are initial target state and final positronium state, respectively. We

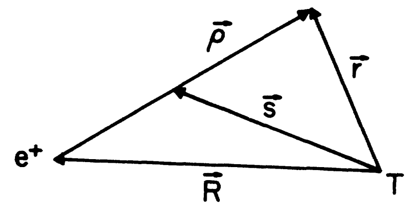

FIG. 1. Coordinates for a positron e^+, colliding with a target of an electron e and a nucleus Z_T.

take the active electron to be initially in the 1s state and the positronium is in the nlm state. Then

$$\psi_i = \Phi_{1s}(\mathbf{r}) e^{i\mathbf{K}_i\cdot\mathbf{R}} \tag{4}$$

and

$$\psi_f = \Phi'_{nlm}(\boldsymbol{\rho}) e^{i\mathbf{K}_f\cdot\mathbf{S}}$$

satisfy the equations

$$H_i\psi_i = (\tfrac{1}{2}K_i^2 + \varepsilon_{1s})\psi_i = E\psi_i \tag{5a}$$

and

$$H_f\psi_f = \left[\frac{1}{2M}K_f^2 + \varepsilon'_n\right]\psi_f = E\psi_f \ , \tag{5b}$$

ε_{1s} and ε'_n being the eigenenergies of the hydrogenic ground state and the positronium nlm state, respectively.

The matrix element in Eq. (3) can be broken into three parts as follows:

$$\begin{aligned} T &= \left\langle \psi_f \left| \left[\frac{Z_T}{R} - \frac{Z_T}{r}\right] \left[1 + G^+ \left[\frac{Z_T}{R}\right]\right] \right| \psi_i \right\rangle \\ &\quad + \left\langle \psi_f \left| \left[\frac{Z_T}{R} - \frac{Z_T}{r}\right] \left[1 + G^+ \left[\frac{-1}{\rho}\right]\right] \right| \psi_i \right\rangle \\ &\quad - \left\langle \psi_f \left| \left[\frac{Z_T}{R} - \frac{Z_T}{r}\right] \right| \psi_i \right\rangle \\ &= T_1 + T_2 - T_3 \ . \end{aligned} \tag{6}$$

The term $T_1 - T_3$ consists[14] of two second-order distortion terms which are new, and T_2 contains two second-order terms which carry Thomas-type singularities.

Evaluation of T_1. To evaluate T_1 we note that

$$\left[1 + G^+\left[\frac{Z_T}{R}\right]\right]\psi_i = \left[1 + \frac{1}{E - \left[-\frac{1}{2}\nabla_R^2 + \varepsilon_{1s} + \dfrac{Z_T}{R} - \dfrac{1}{\rho}\right] + i\eta}\left[\frac{Z_T}{R}\right]\right]\Phi_{1s}(r) e^{i\mathbf{K}_i\cdot\mathbf{R}} \ . \tag{7}$$

We now neglect the potential $(-1/\rho)$ from the Green's function. Equation (7) then takes the form

$$\left[1 + G^+\left[\frac{Z_T}{R}\right]\right]\psi_i \approx \left[1 + \frac{1}{E' - \left[-\frac{1}{2}\nabla_R^2 + \dfrac{Z_T}{R}\right] + i\eta}\left[\frac{Z_T}{R}\right]\right] e^{i\mathbf{K}_i\cdot\mathbf{R}}\Phi_{1s}(r) = \chi_c^+(\mathbf{K}_i,\mathbf{R})\Phi_{1s}(r) \ , \tag{8}$$

where $E' = E - \varepsilon_{1s} = \frac{1}{2}K_i^2$ and $\chi_C^+(\mathbf{K}_i,\mathbf{R})$ is the on-shell Coulomb wave function given by

$$\begin{aligned} \chi_C^+(\mathbf{K}_i,\mathbf{R}) &= e^{-\pi\beta/2}\Gamma(1+i\beta) e^{i\mathbf{K}_i\cdot\mathbf{R}} \\ &\quad \times {}_1F_1(-i\beta, 1; i(K_iR - \mathbf{K}_i\cdot\mathbf{R})) \ , \end{aligned} \tag{9}$$

with $\beta = \mu Z_T / K_i$. Using the result in Eq. (8) we can write

$$\begin{aligned} T_1 &= \left\langle \psi_f \left| \frac{Z_T}{R} - \frac{Z_T}{r} \right| \chi_C^+(\mathbf{K}_i\cdot\mathbf{R})\Phi_{1s}(r) \right\rangle \\ &= T_1^{(R)} - T_1^{(r)} \ , \end{aligned} \tag{10}$$

where $T_1^{(R)}$ and $T_1^{(r)}$ are the matrix elements with interactions Z_T/R and Z_T/r, respectively. We shall now show the evaluation of $T_1^{(r)}$ only, because the evaluation of $T_1^{(R)}$ is very similar to that of $T_1^{(r)}$.

The initial hydrogenic state

$$\Phi_{1s}(r) = \frac{(Z_T)^{3/2}}{\sqrt{\pi}} e^{-\lambda r} \quad \text{with } \lambda = Z_T \ , \tag{11a}$$

and the final positronium state which we take to be a ground state

$$\Phi'_{nlm}(\rho) = \Phi'_{1s}(\rho) = \frac{\beta_1^{3/2}}{\sqrt{\pi}} e^{-\beta_1\rho} \quad \text{with } \beta_1 = \tfrac{1}{2} \ . \tag{11b}$$

For the evaluation of $T_1^{(r)}$ we now use the integral representation[15]

$${}_1F_1(i\alpha, 1, x) = \frac{1}{2\pi i}\oint_\Gamma^{(0^+,1^+)} p(\alpha,t) e^{xt} dt \tag{11c}$$

with

$$p(\alpha,t) = t^{i\alpha-1}(t-1)^{-i\alpha} \ ,$$

where Γ is a closed contour encircling the points 0 and 1 once counterclockwise. Using Eqs. (11a), (11b), and (11c) we arrive at

$$\begin{aligned} T_1^{(r)} = \lim_{\varepsilon\to 0} \frac{c}{2\pi i} \int\int \oint_\Gamma^{(0^+,1^+)} & \frac{e^{-\beta_1\rho - \alpha R - \lambda r}}{r} \\ & \times e^{-i\mathbf{K}_f\cdot\mathbf{S} + i(1-t)\mathbf{K}_i\cdot\mathbf{R}} \\ & \times p(-\beta,t) d\mathbf{r}\, d\mathbf{R}\, dt \ , \end{aligned} \tag{12}$$

where $\alpha = iK_i t + \varepsilon$, and

$$c = \frac{e^{-\pi\beta/2}\Gamma(1+i\beta)Z_T(\beta_1 Z_T)^{3/2}}{\pi} . \tag{13}$$

Performing the space integrations we get

$$T_1^{(r)} = \frac{8c}{2\pi i} \lim_{\varepsilon\to 0} \frac{\partial}{\partial\varepsilon}\frac{\partial}{\partial\beta_1} \oint_\Gamma^{(0^+,1^+)} L(t) p(-\beta,t)dt , \tag{14}$$

where $L(t)$ is the Lewis integral[16]

$$L(t) = \int \frac{d\mathbf{T}}{[(\mathbf{T}-\mathbf{K}_f/2)^2+\beta_1^2](T^2+\lambda^2)\{[\mathbf{T}-\mathbf{K}_f+(1-t)\mathbf{K}_i]^2+\alpha^2\}} = \frac{\pi^2}{(V^2-UW)^{1/2}} \ln\frac{V+(V^2-UW)^{1/2}}{V-(V^2-UW)^{1/2}} \tag{15}$$

with

$$V = \lambda\{[\mathbf{K}_i(1-t)-\mathbf{K}_f/2]^2+(\beta_1+\alpha)^2\} + \alpha(\lambda^2+K_f^2/4+\beta_1^2) + \beta_1\{\lambda^2+\alpha^2+[\mathbf{K}_f-(1-t)\mathbf{K}_i]^2\} ,$$

$$UW = \{[\mathbf{K}_i(1-t)-\mathbf{K}_f/2]^2+(\beta_1+\alpha)^2\} \times [K_f^2/4+(\lambda+\beta_1)^2]\{[\mathbf{K}_f-(1-t)\mathbf{K}_i]^2+(\lambda+\alpha)^2\} .$$

Here we note that the result in Eq. (15) depends on the product UW, not on U and W separately.

We now use the following integral representation[16] for L:

$$L = 2\pi^2 \int_0^\infty dv\,(Uv^2+2Vv+W)^{-1} , \tag{16}$$

where we have split the product UW in such a way that both U and W are linear functions of t. We choose

$$U = [\mathbf{K}_i(1-t)-\mathbf{K}_f/2]^2+(\beta_1+\alpha)^2 ,$$

$$W = [K_f^2/4+(\lambda+\beta_1)^2]\{[\mathbf{K}_f-(1-t)\mathbf{K}_i]^2+(\lambda+\alpha)^2\} .$$

To evaluate the contour integral over Γ we now write

$$U = A + Bt , \quad V = P + Qt , \quad W = E + Ft , \tag{17}$$

where A, B, P, Q, E, and F are functions of K_i, K_f, λ, β_1, and α. Substituting Eqs. (16) and (17) in Eq. (14), we get

$$T_1^{(r)} = 16\pi^2 c \int_0^\infty dv \left[\lim_{\varepsilon\to 0} \frac{\partial}{\partial\varepsilon}\frac{\partial}{\partial\beta_1} \frac{1}{2\pi i} \oint_\Gamma \frac{p(-\beta,t)dt}{G-Ht} \right] , \tag{18}$$

where $G = Av^2+2Pv+E$ and $H = -(Bv^2+2Qv+F)$. Here we note that the t integrand vanishes at $|t| \to \infty$ and the integrand has a pole at $t = G/H$ which is outside the contour Γ. So we can write (see Fig. 2)

$$\oint_\Gamma \frac{p(-\beta,t)dt}{G-Ht} = -2\pi i \,\mathrm{Res}(t = G/H) ,$$

and we finally arrive at

$$T_1^{(r)} = 16\pi^2 c \int_0^\infty \lim_{\varepsilon\to 0} \left[\frac{\partial}{\partial\varepsilon}\frac{\partial}{\partial\beta_1} X(G,H) \right] dv , \tag{19}$$

where

$$X(G,H) = G^{-i\beta-1}(G-H)^{i\beta} . \tag{20}$$

Similarly, the matrix element $T_1^{(R)}$ in Eq. (10) can be evaluated and we obtain

$$T_1^{(R)} = 16\pi^2 c \int_0^\infty \left[\frac{\partial}{\partial\lambda}\frac{\partial}{\partial\beta_1} \lim_{\varepsilon\to 0} X(G,H) \right] dv . \tag{21}$$

It is to be noted that the parameter ε can be put equal to zero in Eq. (19) after differentiating with respect to ε, whereas in Eq. (21) one can put $\varepsilon = 0$ before preforming the derivatives.

Reduction of the matrix element T_2. From Eq. (6) we have

$$T_2 = \left\langle \psi_f \left| \left[\frac{Z_T}{R} - \frac{Z_T}{r} \right] \left[1 + G^+ \left[-\frac{1}{\rho} \right] \right] \right| \psi_i \right\rangle . \tag{22}$$

Now we have

$$\left[1+G^+\left[-\frac{1}{\rho}\right]\right]\psi_i = \left[1+G^+\left[-\frac{1}{\rho}\right]\right]\Phi_{1s}(r)e^{i\mathbf{K}_i\cdot\mathbf{R}}$$

$$= \left[1+\frac{1}{E-H+i\eta}\left[-\frac{1}{\rho}\right]\right]\frac{e^{i\mathbf{K}_i\cdot\mathbf{R}}}{(2\pi)^{3/2}}\int \tilde{\Phi}_{1s}(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{r}}d^3p$$

$$= \left[1+\frac{1}{E-(H_f+V_f)+i\eta}\left[-\frac{1}{\rho}\right]\right]\frac{e^{i\mathbf{K}_i\cdot[\mathbf{S}-(1/2)\rho]}}{(2\pi)^{3/2}}\int \tilde{\Phi}_{1s}(\mathbf{p})e^{i\mathbf{p}\cdot[(1/2)\rho+\mathbf{S}]}d^3p ,$$

where we have changed coordinate $\mathbf{R}$ to $\mathbf{S}-\frac{1}{2}\boldsymbol{\rho}$ and $\mathbf{r}$ to $\frac{1}{2}\boldsymbol{\rho}+\mathbf{S}$. We now ignore $V_f=Z_T/R-Z_T/r$ from G^+ and obtain

$$\left[1+G^+\left[-\frac{1}{\rho}\right]\right]\psi_i=\frac{1}{(2\pi)^{3/2}}e^{i(\mathbf{K}_i+\mathbf{p})\cdot\mathbf{S}}\int\tilde{\Phi}_{1s}(\mathbf{p})\chi^+_{C,\varepsilon',(1/2)(\mathbf{p}-\mathbf{K}_i)}(\boldsymbol{\rho})d^3p\ , \tag{23}$$

where we define

$$\chi^+_{C,\varepsilon',(1/2)(\mathbf{p}-\mathbf{K}_i)}(\boldsymbol{\rho})=\left[1+\frac{1}{\varepsilon'-\left[-\frac{1}{2\mu}\nabla^2_\rho-\frac{1}{\rho}\right]+i\eta}\right]e^{i(1/2)(\mathbf{p}-\mathbf{K}_i)} \tag{24}$$

as the off-shell Coulomb wave function with $\varepsilon'=E-(1/2M)(\mathbf{K}_i+\mathbf{p})^2$. Here we note that on-shell condition is satisfied approximately if

$$\varepsilon'=E-\frac{1}{2M}(\mathbf{K}_i+\mathbf{p})^2\approx\frac{1}{2\mu}[\tfrac{1}{2}(\mathbf{p}-\mathbf{K}_i)]^2$$

or

$$E\approx\tfrac{1}{4}(\mathbf{K}_i+\mathbf{p})^2+\tfrac{1}{4}(\mathbf{p}-\mathbf{K}_i)^2=\tfrac{1}{2}(p^2+K_i^2)\ .$$

Now for the on-shell $E=\frac{1}{2}K_i^2+\varepsilon_{1s}$. The off-shell energy $\frac{1}{2}(p^2+K_i^2)$ thus slightly deviates from the on-shell energy when $\frac{1}{2}p^2$, which is small compared to $\frac{1}{2}K_i^2$, i.e., when

$$\tfrac{1}{2}K_i^2 \gg |\varepsilon_{1s}|\ ,$$

we have the near on-shell condition satisfied. Using Eq. (23) in Eq. (22) and writing $d^3r\,d^3R=d^3\rho\,d^3S$ (since the Jacobian is 1), we arrive at

$$T_2=\frac{Z_T}{(2\pi)^{3/2}}\int\int\int[\Phi'_{nlm}(\boldsymbol{\rho})]^*e^{-i\mathbf{K}_f\cdot\mathbf{S}}\left[\frac{1}{|\mathbf{S}-\frac{1}{2}\boldsymbol{\rho}|}-\frac{1}{|\mathbf{S}+\frac{1}{2}\boldsymbol{\rho}|}\right]\chi^+_{C\varepsilon',(1/2)(\mathbf{p}-\mathbf{K}_i)}(\boldsymbol{\rho})e^{i(\mathbf{p}+\mathbf{K}_i)\cdot\mathbf{S}}d^3\rho\,d^3S\,\tilde{\Phi}_{1s}(\mathbf{p})d^3p\ . \tag{25}$$

The integral over $\mathbf{S}$ in Eq. (25) can be evaluated as

$$\int e^{i(\mathbf{K}_i-\mathbf{K}_f+\mathbf{p})\cdot\mathbf{S}}\frac{1}{|\mathbf{S}\pm\frac{1}{2}\boldsymbol{\rho}|}d^3S=4\pi\frac{e^{\mp i(1/2)(\mathbf{K}_i-\mathbf{K}_f+\mathbf{p})\cdot\boldsymbol{\rho}}}{|\mathbf{K}_i-\mathbf{K}_f+\mathbf{p}|^2}\ . \tag{26}$$

Substituting this result in Eq. (25) we get

$$T_2=Z_T\left[\frac{2}{\pi}\right]^{1/2}\int\left[\int d^3\rho[\Phi'_{nlm}(\boldsymbol{\rho})]^*(e^{(i/2)(\mathbf{K}_i-\mathbf{K}_f+\mathbf{p})\cdot\boldsymbol{\rho}}-e^{-(i/2)(\mathbf{K}_i-\mathbf{K}_f+\mathbf{p})\cdot\boldsymbol{\rho}})\chi^+_{C,\varepsilon',(1/2)(\mathbf{p}-\mathbf{K}_i)}(\boldsymbol{\rho})\right]\frac{\tilde{\Phi}_{1s}(\mathbf{p})d^3p}{|\mathbf{K}_i-\mathbf{K}_f+\mathbf{p}|^2}\ . \tag{27}$$

Following McDowell and Coleman[17] the integration over $\boldsymbol{\rho}$ in Eq. (27) can be evaluated to obtain

$$T_2=-\sqrt{32\pi}Z_TN_f\int d^3p\,\tilde{\Phi}_{1s}(\mathbf{p})\frac{\pi\nu e^{\pi\nu}}{\sinh(\pi\nu)}\frac{1}{|\mathbf{J}+\mathbf{P}|^2}\left[\frac{\frac{1}{2}p^2+|\varepsilon_{1s}|}{(\mathbf{v}-\mathbf{p})^2}\right]^{-i\nu}$$
$$\times\frac{\partial}{\partial\beta_1}(\{\tfrac{1}{4}[(2\beta_1-iv)^2+J^2+2\mathbf{p}\cdot(\mathbf{J}+\mathbf{v}+2i\beta_1\tilde{\mathbf{v}})]\}^{-i\nu}\{[\beta_1^2+(\tilde{\mathbf{v}}-\mathbf{p})^2]^{-1+i\nu}$$
$$-(\beta_1^2+K^2)^{-1+i\nu}\})\ , \tag{28}$$

where we have considered that the final positronium state is the $1s$ state, as in Eq. (11b), and

$$N_f=\frac{\beta_1^{3/2}}{\sqrt{\pi}}\ ,$$

$$\nu=\frac{1}{|\mathbf{v}-\mathbf{p}|},\quad \beta_1=\tfrac{1}{2},\quad \tilde{\mathbf{v}}=\tfrac{1}{2}\mathbf{K}_f,\quad \mathbf{v}=\mathbf{K}_i\ ,$$
$$\mathbf{K}=\tfrac{1}{2}\mathbf{K}_f-\mathbf{K}_i,\quad \mathbf{J}=\mathbf{K}_i-\mathbf{K}_f,\quad \mathbf{J}+\mathbf{K}+\tilde{\mathbf{v}}=0\ .$$

Keeping the term

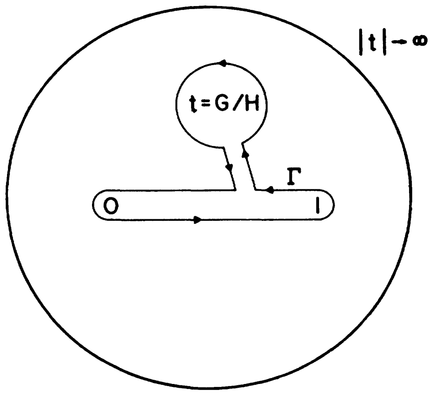

FIG. 2. Illustration of the contour Γ in Eq. (11c) with the pole point $t=G/H$ of the integrand in Eq. (18).

$$G=\tfrac{1}{4}[(2\beta_1-iv)^2+J^2+2\mathbf{p}\cdot(\mathbf{J}+\mathbf{v}+2i\beta_1\hat{\mathbf{v}})] \tag{29}$$

in Eq. (28) unaltered, we then expand other $\mathbf{p}$ dependent terms in powers of p/v, following closely the method of Sil and McGuire.[10] The various expanded terms are

$$\nu=\frac{1}{|\mathbf{V}-\mathbf{p}|}\approx\nu_1(1+x),\quad \nu_1=1/v,\quad x=\mathbf{p}\cdot\mathbf{v}/v^2\ ,$$

$$\frac{1}{|\mathbf{J}+\mathbf{p}|^2}\approx\frac{1}{J^2+p^2}(1-2y),\quad y=\mathbf{J}\cdot\mathbf{p}/(J^2+p^2)\ ,$$

$$\frac{\nu e^{\pi\nu}}{\sinh(\pi\nu)}=h_0+h_1x\ ,\quad h_0=\frac{2\nu_1}{1-e^{-2\pi\nu_1}}\ ,$$

$$h_1=h_0\left[1-\frac{2\pi\nu_1 e^{-2\pi\nu_1}}{1-e^{-2\pi\nu_1}}\right],$$

$$\left[\frac{G}{(\mathbf{v}-\mathbf{p})^2[\beta_1^2+(\tilde{\mathbf{v}}-\mathbf{p})^2]}\right]^{-i\nu}\frac{1}{\beta^2+(\tilde{\mathbf{v}}-\mathbf{p})^2}$$
$$=v^{2i\nu_1}(\beta_1^2+\tilde{v}^{\,2})^{i\nu_1-1}G^{-i\nu_1}$$
$$\times\left[1+2x'(1-i\nu_1)-i\nu_1x\left[\ln\frac{G}{v^2(\tilde{v}^{\,2}+\beta_1^2)}+2\right]\right],$$

$$x'=\mathbf{p}\cdot\tilde{\mathbf{v}}/(\beta_1^2+\tilde{v}^{\,2})\ ,$$

and

$$\left[\frac{G}{(\mathbf{v}-\mathbf{p})^2(\beta_1^2+K^2)}\right]^{-i\nu}\frac{1}{(\beta_1^2+K^2)}$$
$$=v^{2i\nu_1}(\beta_1^2+K^2)^{i\nu_1-1}$$
$$\times G^{-i\nu_1}\left[1-2i\nu_1-ix\nu_1\ln\frac{G}{v^2(\beta_1^2+K^2)}\right]. \tag{30}$$

We now substitute all these expressions in Eq. (28) and perform the derivative with respect to β_1. Terms through first order in p/v then give us

$$\begin{aligned}T_2^{(1)}=\int d^3p\,f'(p)\Bigg[&a'_{10}G^{-i\nu_1}+a'_{20}G^{-i\nu_1-1}+a'_{30}(\mathbf{p}\cdot\hat{\mathbf{v}})G^{-i\nu_1-1}+a'_{1x}\left[\frac{\mathbf{p}\cdot\mathbf{v}}{v^2}\right]G^{-i\nu_1}\\
&+a'_{2x}\left[\frac{\mathbf{p}\cdot\mathbf{v}}{v^2}\right]G^{-i\nu_1-1}+a'_{3x}\left[\frac{\mathbf{p}\cdot\mathbf{v}}{v^2}\right](\mathbf{p}\cdot\hat{\mathbf{v}})G^{-i\nu_1-1}+a'_{1y}\left[\frac{\mathbf{p}\cdot\mathbf{J}}{J^2+p^2}\right]G^{-i\nu_1}+a'_{2y}\left[\frac{\mathbf{p}\cdot\mathbf{J}}{J^2+p^2}\right]G^{-i\nu_1-1}\\
&+a'_{3y}\left[\frac{\mathbf{p}\cdot\mathbf{J}}{J^2+p^2}\right](\mathbf{p}\cdot\hat{\mathbf{v}})G^{-i\nu_1-1}+a'_{1z}\left[\frac{\mathbf{p}\cdot\tilde{\mathbf{v}}}{\beta_1^2+\tilde{v}^{\,2}}\right]G^{-i\nu_1}+a'_{2z}\left[\frac{\mathbf{p}\cdot\tilde{\mathbf{v}}}{\beta_1^2+\tilde{v}^{\,2}}\right]G^{-i\nu_1-1}\\
&+a'_{3z}\left[\frac{\mathbf{p}\cdot\tilde{\mathbf{v}}}{\beta^2+\tilde{v}^{\,2}}\right](\mathbf{p}\cdot\hat{\mathbf{v}})G^{-i\nu_1-1}+a'_{1x\,\ln G}\left[\frac{\mathbf{p}\cdot\mathbf{v}}{v^2}\right](\ln G)G^{-i\nu_1}+a'_{2x\,\ln G}\left[\frac{\mathbf{p}\cdot\mathbf{v}}{v^2}\right](\ln G)G^{-i\nu_1-1}\\
&+a'_{3x\,\ln G}\left[\frac{\mathbf{p}\cdot\mathbf{v}}{v^2}\right](\mathbf{p}\cdot\hat{\mathbf{v}})(\ln G)G^{-i\nu_1-1}\Bigg]\ ,\end{aligned} \tag{31}$$

where

$$f'(p)=-\sqrt{32\pi}Z_TN_f\pi\tilde{\Phi}_{1s}(\mathbf{p})\left[\frac{p^2+p_0^2}{2v^2}\right]^{-i\nu_1}(J^2+p^2)^{-1}\ , \tag{32}$$

$$\tilde{\Phi}_{1s}(\mathbf{p})=\frac{2\sqrt{2}}{\pi}p_0^{5/2}(p^2+p_0^2)^{-2}\ ,$$

$$a'_{10}=2h_0\beta_1(i\nu_1-1)F_1\ ,$$

$$a'_{20}=-i\nu_1h_0(2\beta_1-iv)F_2\ ,$$

$$a'_{30}=\nu_1h_0F_2\ ,$$

$$a'_{1x}=2\beta_1(i\nu_1-1)[(\beta_1^2+\tilde{v}^{\,2})^{i\nu_1-2}F_3-(\beta_1^2+K^2)^{i\nu_1-2}F_4]\ ,$$

$$a'_{2x}=-i\nu(2\beta_1-iv)[(\beta_1^2+\tilde{v}^{\,2})^{i\nu_1-1}F_3-(\beta_1^2+K^2)^{i\nu_1-1}F_4]\ ,$$

$$a'_{3x}=\nu_1[(\beta_1^2+\tilde{v}^{\,2})^{i\nu_1-1}F_3-(\beta_1^2+K^2)^{i\nu_1-1}F_4]\ ,$$

$$a'_{1y}=-4h_0\beta_1(i\nu_1-1)F_1\ ,$$

$$a'_{2y}=2i\nu_1h_0(2\beta_1-iv)F_2\ ,$$

$$a'_{3y}=-2h_0\nu_1F_2\ ,$$

$$a'_{1z}=4\beta_1h_0(i\nu_1-1)(2-i\nu_1)(\beta_1^2+\tilde{v}^{\,2})^{i\nu_1-2}\ ,$$

$$a'_{2z}=-2h_0i\nu_1(1-i\nu_1)(2\beta_1-iv)(\beta_1^2+\tilde{v}^{\,2})^{i\nu_1-1}\ ,$$

$$a'_{3z}=2h_0\nu_1(1-i\nu_1)(\beta_1^2-i\tilde{v}^{\,2})^{i\nu_1-1}\ ,$$

$$
\begin{aligned}
&a'_{1x\,\ln G} = -2i\nu_1 h_0 \beta_1 (i\nu_1 - 1) F_1 \,, \\
&a'_{2x\,\ln G} = -\nu_1^2 h_0 (2\beta_1 - iv) F_2 \,, \\
&a'_{3x\,\ln G} = -i\nu_1^2 h_0 F_2 \,, \\
&F_1 = (\beta_1^2 + \tilde{v}^2)^{i\nu_1 - 2} - (\beta_1^2 + K^2)^{i\nu_1 - 2} \,, \\
&F_2 = (\beta_1^2 + \tilde{v}^2)^{i\nu_1 - 1} - (\beta_1^2 + K^2)^{i\nu_1 - 1} \,, \\
&F_3 = i\nu_1 h_0 [\ln v^2 (\tilde{v}^2 + \beta_1^2) - 2] + h_1 \,, \\
&F_4 = i\nu_1 h_0 [\ln v^2 (\beta_1^2 + K^2) - 2] + h_1 \,.
\end{aligned} \tag{33}
$$

The angular integration in Eq. (31) is then carried out following the method of SM and we finally obtain

$$T_2^{(1)} = \sum_{k=1}^{3} \sum_{j=0,x,y,z,x\,\ln G} \int_0^\infty dp\, p^2 f'(p) a'_{kj} 2\pi \mathcal{J}'_{kj} \,, \tag{34}$$

where $f'(p)$ and a'_{kj} are defined in Eqs. (32) and (33). To obtain $\mathcal{J}'_{kj}$ terms we note that the summation in Eq. (34) contains three new terms compared to $\mathcal{J}_{kj}$ terms in Eq. (3.17) of SM. These new terms are $\mathcal{J}'_{1z}$, $\mathcal{J}'_{2z}$ and $\mathcal{J}'_{3z}$. However, the expressions for these terms can be obtained from the expressions of $\mathcal{J}_{1x}$, $\mathcal{J}_{2x}$, and $\mathcal{J}_{3x}$, respectively, replacing $\mathbf{L}\cdot\mathbf{v}$ by $\mathbf{L}'\cdot\tilde{\mathbf{v}}$ and v^2 by $\tilde{v}^2+\beta_1^2$. For $\mathcal{J}'_{1y}$, $\mathcal{J}'_{2y}$, and $\mathcal{J}'_{3y}$ we use the corresponding expressions of SM with $\mathbf{K}$ replaced by $\mathbf{J}$ and K^2 by J^2+p^2. The expressions for other $\mathcal{J}'_{kj}$ are similar to those of $\mathcal{J}_{kj}$ in SM. We further note that the parameters A and L appearing in the expressions of $\mathcal{J}_{kj}$ are to be replaced by A' and L' and the T functions in $\mathcal{J}_{kj}$ correspond to G functions in the present calculation, where

$$G = A' + 2\mathbf{L}'\cdot\mathbf{p} \,,$$

with

$$
\begin{aligned}
&A' = \tfrac{1}{4}[(2\beta_1 - iv)^2 + J^2] \,, \\
&\mathbf{L}' = \tfrac{1}{4}(\mathbf{J} + \mathbf{v} + 2i\beta_1 \hat{v}) \,,
\end{aligned} \tag{35}
$$

and

$$L' = (\mathbf{L}'\cdot\mathbf{L}')^{1/2} \,.$$

To obtain the zeroth-order terms in T_2 (i.e., $T_2^{(0)}$), one has to take $j=0$ terms only corresponding to the second summation in (34). Here we would point out that $T_2^{(0)}$ can be evaluated analytically following Deb *et al.*[18]

The evaluation $T_2^{(1)}$ in Eq. (34) is thus complete through first order in p/v. The numerical integration over p is to be carried out in a similar way as was done by SM where a term with one Thomas singularity is considered. Here the cancellation of the two Thomas singularities occurs in the F_1 term of Eq. (33) at 45°.

Evaluation of T_3. T_3 is a first-Born-type matrix element with the interaction $(Z_T/R - Z_T/r)$. We write

$$
\begin{aligned}
T_3 &= \left\langle \psi_f \left| \frac{Z_T}{R} - \frac{Z_T}{r} \right| \psi_i \right\rangle \\
&= T_3^{(R)} - T_3^{(r)} \,.
\end{aligned} \tag{36}
$$

$T_3^{(R)}$ can be evaluated as a double derivative of a Lewis[16] integral as follows:

$$T_3^{(R)} = \frac{8\pi^2 Z_T (Z_T\beta_1)^{3/2}}{\pi} \frac{\partial}{\partial\lambda} \frac{\partial}{\partial\beta_1} L(U_1, V_1, W_1) \,, \tag{37}$$

where

$$
\begin{aligned}
&L(U_1, V_1, W_1) \\
&\quad = (V_1^2 - U_1 W_1)^{-1/2} \ln \frac{V_1 + (V_1^2 - U_1 W_1)^{1/2}}{V_1 - (V_1^2 - U_1 W_1)^{1/2}} \,,
\end{aligned} \tag{38}
$$

with

$$
\begin{aligned}
&U_1 = K_i^2 + K_f^2/4 - \mathbf{K}_i\cdot\mathbf{K}_f + \beta_1^2 \,, \\
&V_1 = \lambda(K_i^2 + K_f^2/4 - \mathbf{K}_i\cdot\mathbf{K}_f + \beta_1^2) \\
&\qquad + \beta_1(\lambda^2 + K_i^2 + K_f^2 - 2\mathbf{K}_i\cdot\mathbf{K}_f) \,, \\
&W_1 = (K_f^2/4 + \lambda^2 + 2\lambda\beta_1 + \beta_1^2)(K_i^2 + K_f^2 - 2\mathbf{K}_i\cdot\mathbf{K}_f + \lambda^2) \,,
\end{aligned} \tag{39}
$$

and $T_3^{(r)}$ is given by

$$T_3^{(r)} = \frac{32\pi^2 (Z_T\beta_1)^{5/2}}{[(\mathbf{K}_i - \mathbf{K}_f/2)^2 + \beta_1^2]^2 [(\mathbf{K}_i - \mathbf{K}_f)^2 + \lambda^2]} \,. \tag{40}$$

III. RESULTS

Applying our technique described in Sec. II we have calculated the 1*s*-1*s* differential and total cross sections at several energies for the $e^+ + \mathrm{H}$ system. In Figs. 3 and 4 we present the differential cross sections at $v=10$ and 20 a.u., respectively. DMS is the present result and BK is the Brinkman-Kramer result. The structure near 45° in the DMS result for $v=20$ a.u. is more prominent than the corresponding structure for $v=10$ a.u. We noticed earlier[14] that this structure is due to the destructive

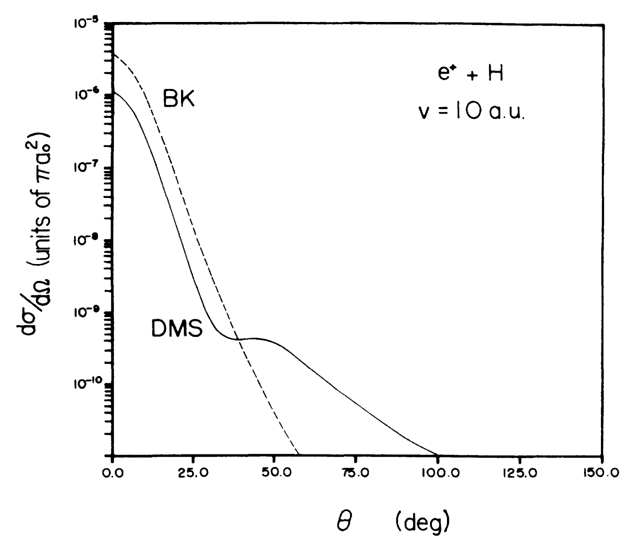

FIG. 3. Differential cross section in units of πa_0^2 at $v=10$ a.u. DMS is our first-order result and BK is the Brinkman-Kramer result.

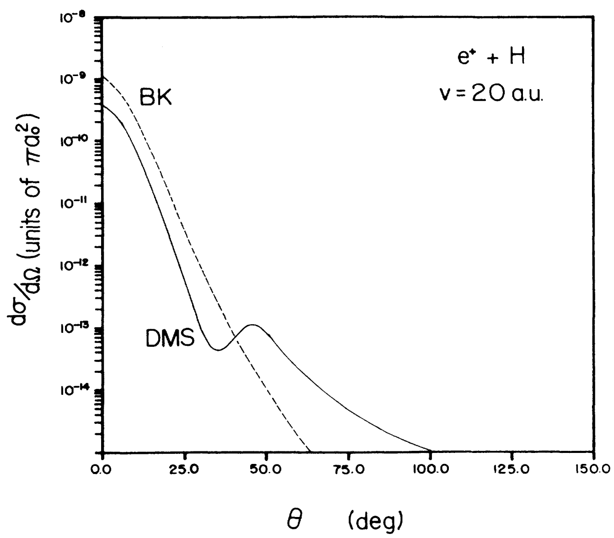

FIG. 4. Same as Fig. 3 at $v=20$ a.u.

interference between T_1 and T_2. For the proton-hydrogen system one normally obtains two peaks: one near $\theta_T=m/M_p\sin 60°$ and other near 60° where $m\,(M_p)$ is the electron (projectile) mass. For the $e^+ + \mathrm{H}$ system, these two peaks approach 45°, and due to the destructive interference of the two amplitudes we get a residual structure. In fact, it is the term (T_1-T_3) that prevents the total cancellation in the differential cross section with the term T_2 that generally happens in first-order theories where there is a dip in the differential cross section near 45°. It is also interesting to note that the BK results are quite a few times larger than the DMS results at forward angles, whereas in the backward angles (not shown), they are several orders of magnitude less than the DMS results. Since most of the contributions to the total cross sections come from the forward angles, the BK total cross section appears to be about three times larger than our DMS result in the energy range considered here.

In Table I we present the total cross sections. $\sigma^{(0)}$ and $\sigma^{(1)}$ are the zeroth- and first-order total cross sections in the present method and $\sigma_{\rm BK}$ is the Brinkman-Kramer result. We also present in Table I the total cross sections for electron capture by protons, $\sigma^{(p+)}$ from the hydrogen atom. Both our results and the BK results differ with $\sigma^{(p+)}$ by at least an order of magnitude at the same velocity. So the ratio for electron capture by positron ($\sigma_{\rm Ps}$) to the electron capture by protons ($\sigma_{\rm H}$) might be informative. It may be worth trying to see how this ratio ($\sigma_{\rm ps}/\sigma_{\rm H}$) behaves as a function of energy as well as target charge.

TABLE I. $\sigma^{(0)}$, $\sigma^{(1)}$, and $\sigma_{\rm BK}$ are the Ps-formation total cross sections (in units of πa_0^2) for zeroth-order (cf. Ref. 14) and first-order terms of present calculation and the Brinkman-Kramer results. $\sigma^{(p+)}$ is the corresponding result for electron capture by protons from the hydrogen atom. The integers in square brackets are the powers of 10 by which the respective numbers are to multiplied.

v (a.u.)	$\sigma^{(0)}$	$\sigma^{(1)}$	$\sigma_{\rm BK}$	$\sigma^{(p+)}$
4	1.94[−3]	1.98[−3]	6.46[−3]	6.16[−5]
6	2.52[−5]	2.57[−5]	9.17[−5]	1.47[−6]
8	1.00[−6]	1.02[−6]	3.66[−6]	7.51[−8]
10	7.83[−8]	7.98[−8]	2.81[−7]	7.07[−9]
14	1.60[−9]	1.62[−9]	5.46[−9]	1.79[−10]
20	2.47[−11]	2.50[−11]	7.97[−11]	3.30[−12]
30	2.08[−13]	2.10[−13]	6.32[−13]	3.29[−14]
50	4.88[−16]	4.92[−16]	1.40[−15]	9.51[−17]
100	1.26[−19]	1.27[−19]	3.43[−19]	3.47[−20]

It is clear from Table I that the first-order cross section $\sigma^{(1)}$ gives a correction of 5% over the zeroth-order contribution $\sigma^{(0)}$. This suggests that zeroth-order calculation is enough, but it may not be true for targets other than hydrogen. Since the effective charge of the target nucleus plays an important role in the kinematics of the problem and hence through the expansion parameter Z_T/v, the first-order contribution may give a correction of more than 5% over the zeroth-order term when Z_T is large.

IV. SUMMARY

In the present paper we present a method for calculating 1s-1s cross sections for Ps formation. Our formulation includes all second-Born terms, including Coulomb distortion terms. Calculations[14] for the singular parts of the amplitude, i.e., the Thomas amplitudes, include positronium intermediate states, whereas the Coulomb distortion term includes hydrogenic intermediate states. The total amplitude is expressed as

$$T=T_1+T_2-T_3\ , \tag{41}$$

where

$$T_1=16\pi^2 c\int_0^\infty\left[\left[\frac{\partial}{\partial\lambda}\frac{\partial}{\partial\beta_1}\lim_{\varepsilon\to0}X(G,H)\right]-\left[\lim_{\varepsilon\to0}\frac{\partial}{\partial\varepsilon}\frac{\partial}{\partial\beta_1}X(G,H)\right]\right]dv\ , \tag{42}$$

with $X(G,H)$ given in Eq. (20),

$$T_3=\frac{8\pi^2 Z_T(Z_T\beta_1)^{3/2}}{\pi}\frac{\partial}{\partial\lambda}\frac{\partial}{\partial\beta_1}L(U_1,V_1,W_1)-\frac{32\pi^2(Z_T\beta_1)^{5/2}}{[(\mathbf{K}_i-\mathbf{K}_f/2)^2+\beta_1^2]^2[(\mathbf{K}_i-\mathbf{K}_f)^2+\lambda^2]}\ , \tag{43}$$

with $L(U_1,V_1,W_1)$, U_1,V_1, and W_1 given in Eqs. (38) and (39). The dominant term (T_2) in the amplitude is first expanded in powers of p/v and then evaluated to (through first order in p/v)

$$T_2^{(1)}=\sum_{k=1}^{3}\sum_{j=0,x,y,z,x\ln G}\int_0^\infty dp\,p^2 f'(p)a'_{kj}2\pi\mathcal{J}'_{kj}\ , \tag{44}$$

where $f'(p)$ and a'_{kj} are given in Eqs. (32) and (33). The terms $\mathcal{J}'_{kj}$ are to be obtained from $\mathcal{J}_{kj}$ in the work of SM, as discussed in the last part of Sec. II [i.e., just after

Eq. (34)]. To use the expressions for $\mathcal{J}_{kj}$ from SM one has to note that A, L, and T in SM should be replaced by A', L', and G, respectively in the present calculation where A', L', and G are given in Eq. (35).

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