Positron annihilation in $e^+ - H$ collision above the Positronium formation threshold

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A long-standing problem to account for the electron-positron annihilation in positron Hydrogen scattering above the Positronium formation threshold has been resolved by the use of the three-body Faddeev formalism. The multichannel three-body theory for scattering states in presence of a complex absorbing potential is developed in order to compute the direct $e^+e^-$ annihilation amplitude, the amplitude of Positronium formation and respective cross sections. A number of $e^+e^-$ direct annihilation cross sections and Positronium formation cross sections in the energy gap between Ps(1s) and H$(n=2)$ thresholds are reported for both the positron-Hydrogen incoming channel as well as the proton-Positronium incoming channel.

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When colliding with the Hydrogen atom in the energy region between Positronium Ps(1s) and Hydrogen H$(n=2)$ thresholds, the positron can annihilate in two possible channels either in the elastic $e^+ - H$ one or in the rearrangement $p^- - Ps$ one. During rearrangement the positron captures the electron from H and forms Positronium in the Ps(1s) state and then the positron-electron pair annihilates from this state. The lifetime of Ps(1s) is known to depend on the total spin $J$. This well known annihilation mechanism is of the two-body nature, i.e., once Positronium is formed the third particle does not affect the annihilation process. The annihilation mechanism in the elastic $e^+ - H$ channel is more complicated and needs three-body footing. There was a number of attempts for the unified three-body treatment of the positron annihilation phenomenon and the Positronium formation, especially in the vicinity of the Positronium formation threshold \cite{1, 2, 3}. Nevertheless as to the best of our knowledge, the self-consistent multichannel theory for the annihilation in positron-atom collisions when the rearrangement channel is open does not exist to date. It is the aim with this paper to fill out this gap by combining the three-body multichannel scattering approach basing on modified Faddeev equations (MFE) \cite{5, 6} with the concept of a complex absorbing potential \cite{2} which allows to treat the annihilation in the framework of non-relativistic quantum mechanics. In the paper we restrict ourselves within the Ore gap energy region. The extension onto the case when more than one Hydrogen (and Positronium) state are participating is straightforward.

Let us recapitulate those portions of the one channel approach to the description of the annihilation phenomenon in positron Hydrogen scattering below the rearrangement threshold which are essential for a multichannel extension. The well known QED formula \cite{7, 8}

\[ \sigma^t = \pi r_0^2(c/v)Z_{\text{eff}} \]  

expresses the spin averaged annihilation cross section $\sigma^t = 1/4^1\sigma^t + 3/4^1\sigma^t$ in terms of the effective number of electrons $Z_{\text{eff}}$ contributing to the annihilation. The respective number $2S+1Z_{\text{eff}}$ for a spin state $S$ is given by the integral

\[ 2S+1Z_{\text{eff}} = \int dr_1 dr_3 |2S+1\Psi^0(r_1, r_3)|^2 \delta(r_1 - r_3). \]  

Throughout the paper we use bold letters for vectors, e.g., $r$, not bold ones for their magnitudes, e.g., $|r|$, and we choose units such that $\hbar = 1$. In formula (1) and (2) the ingredients have the following meaning, $r_0$ is the classical electron radius, $c$ is the velocity of light, $v$ is the incident velocity of positron, $2S+1\Psi^0$ is the $e^+ - H$ scattering wave function when only Coulomb interaction is taken into account, and $r_1$ and $r_3$ are position vectors of positron and electron in the coordinate frame associated with proton. The presence of the delta-function in (2) manifests the fact that $e^+$ and $e^-$ annihilate when they occupy the same position. The non-relativistic quantum mechanical description consistent with the above formulation can be based on the concept of a complex absorbing potential \cite{2}. \cite{3}. The use of this potential in the Schrödinger equation leads to the particle loss. The cross section associated with this loss is actually the annihilation cross section. The absorbing potential is defined by \cite{3}

\[ igW(r_1 - r_3) \equiv -i(e^2/a_0)(2S+1)c\alpha^{S+3}\delta(r_1 - r_3), \]  

where $e$ is the electron charge, $a_0$ is the Bohr radius, $\alpha$ is the fine structure constant, and spin dependent constants $2S+1c$ are defined as $1c = 2\pi$ and $3c = \Sigma(\pi^2 - 9)/9$.

The Schrödinger equation for the positron Hydrogen wave function with outgoing asymptotic boundary conditions

\[ (E - H^0)\Psi_{p_1} = igW\Psi_{p_1}, \]

where $H^0$ is the three-body Coulomb Hamiltonian and $p_1$ is the momentum of incident positron, can be rewritten as

\[ \Psi_{p_1}^+ = \Psi_{p_1}^0 + ig(E^+ - H^0)^{-1}W\Psi_{p_1}^+. \]

Here $\Psi_{p_1}^0$ is the solution to the pure three-body Coulomb problem $(H^0 - E)\Psi_{p_1}^0 = 0$ and $E^+ = E + i0$. It is seen from (4) that the asymptotics of $\Psi_{p_1}^+$, as $r_1$ approaches infinity, takes the form

\[ \Psi_{p_1}^+(r_1, r_3) \sim \psi(r_3)e^{i\int_{r_1}^{r_3} \Psi_{p_1}^+ [F_e - igF_a]} \]  

where $F_e$ and $F_a$ are the electric field and the complex absorbing potential.
In [5], $\psi(p_1)$ is the Hydrogen ground state wave function. The elastic scattering amplitude $F_{e}$ is entirely due to the $\psi_{p_1}^{0+}$ contribution, and the annihilation amplitude $F_{a}$ is due to the absorbing potential. This amplitude is given by

$$F_{a}(p_1', p_1) = \frac{m}{2\pi} (\Psi_{p_1}^{0+}|W|\Psi_{p_1}^{+}),$$  \hspace{1cm} (6)

where $m$ is the electron mass. In principle, the annihilation cross section $\sigma^a$ can be computed from the total cross section $\sigma^t$ as

$$\sigma^a = \sigma^t - \int d\Omega |F_{e}|^2, \quad \sigma^t = \int d\Omega |F_{e} - igF_{a}|^2,$$  \hspace{1cm} (7)

but in the one channel case there is an alternative way which is based on the optical theorem

$$\sigma_a = \frac{4\pi}{p_1} \Im [F_{e}(p_1, p_1) - igF_{a}(p_1, p_1)],$$

from which the annihilation cross section appears as

$$\sigma_a = \frac{4\pi}{p_1} \Im [-iF_{a}(p_1, p_1)].$$  \hspace{1cm} (8)

Now, the annihilation cross section [1] and the formula [2] for the effective number $Z_{eff}$ follow immediately from [3] and [5] with replacing $Ψ_{p_1}$ in [3] by $Ψ_{p_1}^{0+}$ which, considering [4] perturbatively in view of $|g| \ll 1$, is the first order approximation for $Ψ_{p_1}$ i.e., $Ψ_{p_1}^{0+} = Ψ_{p_1}^{0+} + O(g)$. Let us now turn to the case when the Positronium formation channel is open and thus the $e^+ - H$ collision becomes truly multi arrangemental. In this case the integral defined by [2] diverges and the cross section defined by formula [1] is infinite. On the contrary, the exact amplitudes $F_{e}$ and $F_{a}$ defined by [5] are finite (as long as the exact solution to [2] is assumed) due to the effect of the absorbing potential which makes the Positronium binding energy complex. Although the exact amplitudes are well defined, the matrix element [5] cannot remedy the problem with the annihilation cross section. Indeed, the contribution of elastic and rearrangement channels to the optical theorem for the three body system [2] is additive

$$\frac{4\pi}{p_1} \Im [F_{e}(p_1, p_1) - igF_{a}(p_1, p_1)] = \sigma_{11} + \sigma_{21}.$$  \hspace{1cm} (9)

Here $\sigma_{11}$ is the total (elastic plus annihilation) cross section in the $e^+ - H$ channel and $\sigma_{21}$ is the total Positronium formation (and annihilation after Positronium formation) cross section. Since the contribution of the annihilation in the left hand side of [2] is proportional to the matrix element [5] it is apparent that with this quantity the direct annihilation process and the process of the annihilation after Positronium formation are inseparable. We believe that a variant of this effect of inseparability was observed in the numerical study of positron Hydrogen scattering in [3, 10].

So, it is clear that the shortcoming of the outlined formalism is due to an inadequate treatment of multichannel scattering.

The approach which is proven to define correctly the transition amplitudes between all open channels in the three-body case is the Faddeev equation formalism [5] and its modification MFE for long-range interactions [4]. In this approach the wave function is split into the sum of components each of them corresponding to the given asymptotic arrangement. The solution of the set of equations for components (Faddeev equations) satisfies the following requirements: i) the sum of components obeys the Schrödinger equation; ii) the asymptotics of the component associated with a given asymptotic arrangement includes contributions from all open channels in this arrangement and coincides with the restriction of the wave function on this arrangement [6]. This last property guaranties that the amplitudes computed from components are exact physical scattering amplitudes.

The three-body relative Jacobi coordinates $x_i$ and $y_i$ are used to describe the configuration of the three-body system in the c.m. frame. So it is not required for proton to be infinitely heavy. The index $i$ runs over all three arrangements of the system and corresponds to the spectator particle $i$. The positron Hydrogen Hamiltonian reads

$$H = T + \frac{e_1 e_2}{x_1} + \frac{e_3 e_1}{x_2} + \frac{e_1 e_2}{x_3} + igW_{2}(x_2).$$  \hspace{1cm} (10)

Here $T$ is the c.m. kinetic energy, the index 1 corresponds to the positron, whereas 2 and 3 do to proton and electron, respectively, thus $e_1 = e_2 = e, e_3 = -e$. The last term $igW_{2}$ is the absorbing potential [5]. For long-range potentials the modification [6] is needed, which consists in splitting of the Coulomb potentials into long-range $V_{l}^{i}$ and short-range $V_{s}^{i}$ pieces such that

$$V_{l}^{i}(x_i, y_i) + V_{s}^{i}(x_i, y_i) = V_{l}^{iC}(x_i); \quad V_{s}^{i} = V_{s}^{iC} - V_{l}^{i}. \hspace{1cm} (11)

This splitting is made in the three-body configuration space by a smooth splitting function $ζ_{l}(x_i, y_i)$ constructed in such a way that $ζ_{l}(x_i, y_i) = 1$ if $x_i/x_0 = (1 + y_i/y_0)^{y_0}$ and $ζ_{l}(x_i, y_i) = 0$ if $x_i/x_0 > (1 + y_i/y_0)^{y_0}$ for some $x_0 > 0, y_0 > 0$ and $0 < \nu < 1/2$. With such a $ζ_{l}$ the short- and long-range parts of the Coulomb potentials are defined as

$$V_{l}^{iC}(x_i, y_i) = ζ_{l}(x_i, y_i)V_{l}^{iC}(x_i); \quad V_{s}^{i} = V_{s}^{iC} - V_{l}^{i}.$$  \hspace{1cm} (12)

The Hamiltonian [10] is transformed then into

$$H = H^{l} + V_{l}^{i} + V_{s}^{i} + igW_{2}; \quad H^{l} = T^{l} + V_{l}^{i} + V_{l}^{iC}.$$  \hspace{1cm} (13)

Faddeev components of the wave function $Ψ_{i}^{+}$ are defined by formulae

$$Ψ_{1}^{+} = (E^{+} - H^{l})^{-1}V_{l}^{iC}Ψ^{+}$$
$$Ψ_{2}^{+} = (E^{+} - H^{l})^{-1}(V_{s}^{i} + igW_{2})Ψ^{+},$$

where $E^{+} = E + i0$. It is straightforward to see that the sum of the components gives the wave function

$$Ψ^{+} = Ψ_{1}^{+} + Ψ_{2}^{+}.$$  \hspace{1cm} (14)
and the components obey the set of MFE

$$(E - H^l - V_1^s)\Psi_1^- = V_1^s\Psi_2^-,$$
$$(E - H^l - V_2^s - igW_2)\Psi_2^- = (V_2^s + igW_2)\Psi_1^-.$$

(12)

The important feature of equations (12), with regard to description of the annihilation, is the fact that the two-body annihilation potential $igW_2$ is incorporated into equations in two manners, i.e., in the diagonal part on the left hand side of the equation (12) being responsible in the channel 2 for annihilation of Positronium after its formation, and in the coupling term on the right hand side supporting the annihilation process in the positron Hydrogen channel 1 through the coupling.

The set of MFE (12) treats the multichannel nature of the problem above the Positronium formation threshold correctly. Namely, in the asymptotic part of the channel 1 where $|y_1| \to \infty$ and $x_1$ is confined within the Hydrogen atom volume, the only nonvanishing potentials are $V_1^s$ and $V_2^s$ in the combination $V_1^s + V_2^s = V^s$ and the first MFE takes the form

$$(E - T - V^s_1)\Psi_1^+ = 0.$$ 

So, it is obvious that asymptotically

$$\Psi_1^+(x_1, y_1) \sim \phi_1(x_1)e^{iy_1},$$

where $\phi_1(x_1)$ is the Hydrogen wave function with the energy $\epsilon_1$, so that $E = p^2_1/2\mu_1 + \epsilon_1$, and $\nu_1$ is the $e^+ - H$ reduced mass. In the asymptotic part of the channel 2, where $|y_2| \to \infty$ and $x_2$ is confined in the volume of the Positronium atom the nonvanishing potential is $V_2^s + igW_2$ and the second MFE is reduced to

$$(E - T - V^s_2 - igW_2)\Psi_2^+ = 0.$$ 

Hence, the asymptotics of the component $\Psi_2^+$ can be written as

$$\Psi_2^+(x_2, y_2) \sim \phi_2(x_2)e^{ip_2y_2}, \quad E = p^2_2/2\nu_2 + \epsilon_2$$

where $\nu_2$ is the $p$-Ps reduced mass, $\phi_2(x_2)$ is the Positronium wave function in presence of the absorbing potential, i.e., the solution to the equation

$$[-\Delta_{x_2} - \frac{e^2}{x_2} + igW_2(x_2)]\phi_2(x_2) = \epsilon_2\phi_2(x_2).$$

(13)

Let us notice, that the first order approximation with respect to $g$ gives for $\epsilon_2$ the formula

$$\epsilon_2 \sim \epsilon_2^0 + ig[\phi_2^0|W_2|\phi_2^0],$$

with $\epsilon_2^0$ and $\phi_2^0$ defined as the solution to (13) if $g = 0$, i.e., the pure Coulomb problem for Positronium.

The above arguments can be formalized rigorously with the use of integral equations. To this end it is convenient to introduce matrix notations

$$V = \begin{bmatrix} 0 & V_1^s \\ V_2^s & 0 \end{bmatrix}, \quad W = \begin{bmatrix} 0 & 0 \\ W_2 & 0 \end{bmatrix}, \quad I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Thus, the MFE set takes the form

$$[E\Gamma - H(g) - V]\Psi = igW\Psi,$$ 

(14)

where $\Psi = (\Psi_1^+, \Psi_2^-)^T$. The equation (14) can be rewritten as

$$\Psi = \Psi^0 + ig[E\Gamma - H(g) - V]^{-1}W\Psi.$$ 

(15)

Here $\Psi^0$ is the solution to the homogeneous equation

$$[E\Gamma - H(g) - V]\Psi^0 = 0$$ 

(16)

which can be transformed to the integral form

$$\Psi^0 = \Phi + [E\Gamma - H(g)]^{-1}V\Psi^0.$$ 

(17)

The driving term $\Phi$ obeys the homogeneous equation

$$[E\Gamma - H(g)]\Phi = 0$$ 

and its components $\Phi = (\Phi_1, \Phi_2)^T$ are given in terms of channel functions $\phi_i(x_i)$ by formulæ

$$\Phi_i(x_i, y_i) = \phi_i(x_i)e^{ip_iy_\nu}\delta_{ik}$$

which define through the index $k = 1, 2$ of the Kronecker-delta the initial state of the $e^+ - H$ system.

From the analysis made in [5], [6] it follows that matrix integral equations (15) and (17) are well defined and possess the property that the driving term defines the solution uniquely. So that, the asymptotics of the solutions of (15) and (17) is entirely due to the asymptotics of the resolvent operators incorporated in the kernels of these equations. The latter asymptotics can be evaluated with the help of techniques developed in [5], [6], [11] which leads to the following result for the solution to (15) as $y_i \to \infty$

$$\Psi^+_i(x_i, y_i, p_k) \sim \phi_i(x_i)[e^{ip_iy_\nu}\delta_{ik} + \frac{e^{ip_iy_\nu}}{y_i}F_{ik}(p_iy_i, p_k)].$$

The amplitudes $F_{ik}$ have the structure which is similar to that of one channel case [6]

$$F_{ik}(p_i, p_k) = F_{ik}^0(p_i, p_k) - igF_{ik}^1(p_i, p_k).$$

(18)

The first term $F_{ik}^0(p_i, p_k)$ is entirely due to the contribution of $\Psi^0$ in (15) and if $i = k$ then $F_{ik}^0$ is the elastic scattering amplitude whereas $F_{ik}^0$ is the rearrangement amplitude if $i \neq k$. The second term is due to the absorbing potential. The direct annihilation amplitude in the $e^+ - H$ channel $F_{ik}^1$ is given by the formula

$$F_{ik}^1(p_i', p_k) = \frac{\mu_1}{2\pi} \langle \Psi_1^0(p_i') | + \Psi_2^0(p_i') | W_2 | \Psi_1^+(p_k) \rangle.$$
Components $\Psi_{L}^{(1)}(p_{1})$ are solutions to (17), where the energy should be taken on the lower rim to provide incoming boundary conditions, so that $E^{+}$ should be replaced by $E^{-} = E - \delta_{0}$, and the inhomogeneous term is set as $\Phi_{L}(x_{i}, y_{i}) = \phi_{L}(x_{i}) e^{i p_{i} \cdot \delta_{0}}$. The amplitude $F_{2k}$ has the structure similar to that of (13). It plays the role of the correction term either for the Positronium formation amplitude ($k = 1$) or for the elastic amplitude of Positronium-proton scattering ($k = 2$).

Once amplitudes of all processes are determined, the cross sections of interests are defined by integrals

$$\sigma_{1k} = \frac{v_{1}}{v_{k}} \int d\Omega \left| F_{1k}^{0} \right|^{2}; \quad \sigma_{2k} = \frac{v_{2}}{v_{k}} \int d\Omega \left| F_{2k}^{0} - igF_{2k}^{1} \right|^{2}$$

(19)

$$\sigma_{1k}^{0} = \frac{v_{1}}{v_{k}} \int d\Omega \left[ 2g \Im F_{1k}^{0} F_{1k}^{1} + g^{2} \left| F_{1k}^{1} \right|^{2} \right].$$

(20)

Here we have split the total cross section in the channel 1 into two parts similarly to (7), so that $\sigma_{1k}^{0} = \sigma_{1k} + \sigma_{1k}^{0}$, where $\sigma_{1k}$ is the annihilation cross section. Formulae (19), (20) were used for calculations of the direct annihilation cross section $\sigma_{12}$ and the Positronium formation cross section $\sigma_{21}$ for the $e^{+}$—H incoming channel, and the direct annihilation cross section $\sigma_{12}$ and the Hydrogen formation cross section $\sigma_{12}$ when $p—Ps$ is the incoming channel. During the calculation we systematically used the smallness of the constant $g$ of the absorbing potential to simplify amplitudes, namely, from (15) it follows that $\Psi = \Psi^{0} + O(g)$ and from (17) it is immediately seen that $\Psi^{0} = \Psi^{00} + O(g)$, where $\Psi^{00}$ is the solution to (17) when $g = 0$. Hence, the amplitudes and cross sections in the leading order can be calculated with the solution of MFE for the pure three-body Coulomb problem.

In tables below we list results of our calculations for $\sigma_{12}$, $\sigma_{21}$, and $\sigma_{12}$, $\sigma_{21}$ cross sections for total angular momenta $L = 0$, $L = 1$ and $L = 2$ for five values of the energy of the spectator in the Ore gap. All calculations were performed on the base of a quintic spline algorithm for the solution of differential MFE equations from [13]. The numerical error for cross sections was estimated as not exceeding 5% for $\sigma_{12}$ and 10% for $\sigma_{21}$.

As a concluding remark we want to emphasis that the MFE formalism presented here is exact above the Positronium formation threshold, at the same time it is equivalent to the standard one below the Positronium formation threshold [13] and it is also exact for the Positronium ion Ps [14].

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### TABLE I: Ps formation cross section $\sigma_{21}$, H formation cross section $\sigma_{12}$ and direct annihilation cross sections $\sigma_{12}$ and $\sigma_{11}$ for $L = 0$. Momenta $k$ are in units of $1/a_{0}$, and $\sigma$'s are in units of $\pi a_{0}^{2}$.

| $k$ | 0.8000 | 0.8500 | 0.8612 | 0.8615 | 0.8618 |
|-----|--------|--------|--------|--------|--------|
| $\sigma_{21}$ | 0.4965[-2] | 0.5711[-2] | 0.3239[-1] | 0.826[-3] | 0.3259[-2] |
| $\sigma_{12}$ | 0.113[-1] | 0.9300[-2] | 0.4982[-1] | 0.1287[-2] | 0.4972[-2] |
| $\sigma_{11}$ | 0.299[-6] | 0.329[-6] | 0.399[-6] | 0.332[-6] | 0.336[-6] |
| $\sigma_{12}$ | 0.30[-7] | 0.37[-7] | 0.15[-6] | 0.53[-8] | 0.17[-7] |

### TABLE II: As in TAB. I for $L = 1$ with same units.

| $k$ | 0.8000 | 0.8500 | 0.8615 | 0.8632 | 0.8635 |
|-----|--------|--------|--------|--------|--------|
| $\sigma_{21}$ | 0.4793 | 0.5621 | 0.1022[+1] | 0.6847[-1] | 0.4077 |
| $\sigma_{12}$ | 0.3633 | 0.3032 | 0.5167 | 0.3459 [-1] | 0.2059 |
| $\sigma_{11}$ | 0.58[+6] | 0.40[+6] | 0.57[+6] | 0.23[+6] | 0.47[+7] |
| $\sigma_{12}$ | 0.64[-6] | 0.12[-5] | 0.73[-6] | 0.64[-7] | 0.12[-6] |

### TABLE III: Same as in TAB. I for $L = 2$ with same units.

| $k$ | 0.8000 | 0.8500 | 0.8635 | 0.8635 | 0.8635 |
|-----|--------|--------|--------|--------|--------|
| $\sigma_{21}$ | 0.87[+1] | 0.11[+1] | 0.3086 | 0.1788[+1] | 0.1306[+1] |
| $\sigma_{12}$ | 0.3961 | 0.3779 | 0.2425 | 0.5362 | 0.3917 |
| $\sigma_{11}$ | 0.28[-6] | 0.27[-6] | 0.39[-6] | 0.27[-6] | 0.20[-6] |
| $\sigma_{12}$ | 0.99[-6] | 0.12[-5] | 0.11[-6] | 0.19[-5] | 0.58[-6] |

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