Multichannel formalism for positron–hydrogen scattering and annihilation

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Received 24 December 2006, in final form 14 March 2007
Published 30 April 2007
Online at stacks.iop.org/JPhysB/40/1675

Abstract

A problem to account for the direct electron–positron annihilation in positron–hydrogen scattering above the positronium formation threshold has been resolved within the time-independent formalism. The generalization of the optical theorem is derived for the case when an absorption potential is present in the Hamiltonian. With this theorem, the annihilation cross section is fully determined by scattering amplitudes. This allows us to separate out analytically the contribution of the positronium formation effect from the overall annihilation cross section. The rest is determined as the direct annihilation cross section. It is done uniformly below as well as above the positronium formation threshold. The multichannel three-body theory for scattering states in the presence of an imaginary absorption potential is developed in order to compute the direct $e^+e^-$ annihilation amplitude. Special attention has been paid to an accurate definition of the coordinate part of the absorption potential as the properly constructed zero-range potential, which corresponds to the delta function originating from the first-order perturbation theory. The calculated direct annihilation cross section below the positronium formation threshold is in good agreement with the results of other authors. The direct annihilation cross section computed with the formalism of the paper shows nonsingular behaviour at the positronium formation threshold. A number of $e^+e^-$ direct annihilation cross sections and positronium formation cross sections in the energy gap between $\text{Ps}(1s)$ and $\text{H}(n = 2)$ thresholds are reported. A sharp increase in the calculated direct annihilation cross section across the resonant energy is found for all first S- and P-wave Feshbach resonances.
1. Introduction

In positron–hydrogen collision, if the energy is higher than the positronium formation threshold, we have two genuine different asymptotic channels. The positron may go away leaving the hydrogen atom behind in a ground or in an excited state, or the positron and the electron may form a positronium leaving the proton behind. This picture gets modified if we take into account the possibility that the positron and the electron annihilate. In the case of rearrangement scattering, when the positron and the electron form the positronium (Ps) in the 1s state, the positron–electron pair annihilates mostly from this state. The lifetime of the Ps(1s) state depends on the total spin [1]. Direct annihilation occurs without formation of the positronium. In this case, the positron interacts with the electron in the field of the proton only when all the three particles are close to each other. Thus, direct annihilation is a genuine three-body process.

The conventional approach treats e+e− annihilation on the basis of the perturbation theory [2, 3]. The annihilation cross section is proportional to a matrix element of the coalescence operator between scattering states, which are the solutions of the unperturbed three-body Coulomb Hamiltonian. At higher energies, this formalism has difficulties. At the positronium formation threshold, the calculated annihilation cross section becomes infinite. There has been a number of attempts to improve the theory to get a unified treatment of positron annihilation and positronium formation [4–6]. In one approach, to make the lifetime of the e+e− pair finite, an imaginary absorption potential is added to the positron–electron subsystem Hamiltonian [4]. ‘The loss of particles’, due to this potential, is then interpreted as e+e− annihilation. The perturbative QED formula [2, 3] for the positron annihilation cross section suggests the coordinate part of the absorption potential to be the three-dimensional Dirac delta function depending on the relative position vector between the positron and the electron. Subsequently, this kind of absorption potential was used for computing the annihilation cross section above the positronium formation threshold [5, 7, 8]. The three-dimensional delta function is too singular to be an ordinary potential in the Schrödinger equation [9–11]. In the calculations in [4, 5, 7, 8] with the delta potential, this singularity was smoothed out. Nevertheless, the mathematically sound formulation of using the three-dimensional zero-range potentials in three-body Coulombic systems is still needed. It is done in this paper to complete the theory.

The direct annihilation cross section above the positronium formation threshold is the subject of an extensive study [12]. An analysis made in [5, 6] showed that the direct process and annihilation after positronium formation are inseparable. In contrast, the direct cross section was defined and computed successfully below and above the Ps-formation threshold in [8]. This calculation showed no sign of the presence of any threshold behaviour in the energy dependence of the direct annihilation cross section.

This paper is devoted to the study of direct annihilation within the time-independent formalism [13]. In section 2, we define the scattering solution for the e+–H Schrödinger equation in the presence of an absorption potential. Subsequently, the multichannel formalism, which is needed to determine scattering and absorption amplitudes above the positronium formation threshold, is developed. In section 3, we derive the generalization of the optical theorem in the presence of an absorption potential. This optical theorem is used to separate out the cross section of annihilation after positronium formation from the overall absorption cross section. The remaining part is the direct annihilation cross section. The correct form of the zero-range absorption potential is introduced in section 3. Section 4 contains the results of calculations for direct annihilation. Section 5 concludes the paper.

Throughout the paper we use bold letters for vectors, e.g. \( \mathbf{x} \), and non-bold for their magnitudes, e.g. \( x = |\mathbf{x}| \). The unit vector pointing out in the direction of the vector \( \mathbf{y} \) is
denoted by $\tilde{y} = y/y$. In the paper we work with wavefunctions and their components of the form $\Psi(X, p)$, where $X$ stands for the configuration coordinate and $p$ for the momentum of the asymptotic motion. Avoiding overloading of the formulae, we drop very often the configuration space coordinate from the notations of wavefunctions and their components leaving only the momentum explicitly.

2. Three-body scattering formalism

In this section, we apply the three-body multichannel formalism to $e^+–H$ scattering.

2.1. Three-body scattering in the presence of an absorption potential

We consider the three-body problem with an additional imaginary potential which acts between the positron and the electron. If the centre-of-mass motion is removed, the Hamiltonian in the Jacobi coordinate system takes the form

$$H = H^C + igW_2(x_2),$$

$$H^C = H_0 + V_1^C(x_1) + V_2^C(x_2) + V_3^C(x_3),$$

$$H_0 = -\frac{\hbar^2}{2\mu_i} \nabla^2_{x_i} - \frac{\hbar^2}{2v_i} \nabla^2_{y_i}, \quad V_i^C(x_i) = \frac{e_i e_k}{x_i}.$$  

Here we assign numbers 1, 2 and 3 to the positron, the proton and the electron, respectively; therefore, the electric charges are expressed through the unit charge $e$ as $e_1 = e_2 = e, e_3 = -e$. The Jacobi coordinates are defined in terms of particle radius vectors $r_i$ by the standard formulae

$$x_i = r_j - r_k, \quad y_i = r_i - \frac{m_j r_j + m_k r_k}{m_j + m_k},$$

and the reduced masses are given by

$$\mu_i = \frac{m_j m_k}{m_j + m_k}, \quad v_i = \frac{m_i (m_j + m_k)}{m_i + m_j + m_k}.$$  

The potential $igW_2(x_2)$ acting between particles of the pair 2 is defined such that $g$ is real and negative and $W_2(x_2)$ is real and non-negative. In this case, $igW_2$ is an imaginary absorbing potential. We do not specify the coordinate dependence of $W_2$ yet, except of requiring that $W_2$ is short ranged.

The Schrödinger equation for the positron–hydrogen scattering reads

$$\left(H_0 + V_1^C - E\right)\Psi^* = -(V_2^C + V_3^C + igW_2)\Psi^*.$$  

The scattering solution is defined at the real energy $E$ by the asymptotics as $y_1 \to \infty$

$$\Psi^* \propto \phi_1(x_1) \left[ e^{ip_1 \tilde{y}_1} + \frac{e^{ip_1 \tilde{y}_1}}{\tilde{y}_1} F(p_1 \tilde{y}_1, p_1) \right].$$  

Here $\phi_1(x_1)$ is the hydrogen ground-state wavefunction with the energy $\epsilon_1$, and the incident momentum of the positron $p_1$ is related to the energy by the condition $E = \hbar^2/2v_1 p_1^2 + \epsilon_1$. We note that, due to the asymptotics (7) of the wavefunction, the term $V_2^C + V_3^C$ on the right-hand side of equation (6) is always confined into the region of the configuration space where the hydrogen wavefunction $\phi_1(x_1)$ is not negligible. This makes the term $V_2^C + V_3^C$ short-range type, and hence the asymptotics (7) in the coordinate $y_1$ is free from the Coulomb contribution. This property holds true for all equations we deal with in the paper.
Conventionally [14], the scattering amplitude \( F \) can be represented through the wavefunction. It is done by rewriting equation (6) in the integral form and taking the asymptotics \( y_1 \to \infty \). By doing so, we get the Lippmann–Schwinger equation (LSE)

\[
\Psi^*(\mathbf{p}_1) = \Phi_1(\mathbf{p}_1) + G_1(E^+)(V_2^C + V_3^C + i g W_2)\Psi^*(\mathbf{p}_1),
\]

(8)

where \( E^+ = E+i0, \Phi_1(\mathbf{p}_1) = \phi_1(\mathbf{x}_1) e^{i \Phi_1} \) is the solution to the channel Schrödinger equation

\[
(H_0 + V_1^C - E)\Phi_1(\mathbf{p}_1) = 0,
\]

(9)

and \( G_1 \) is the channel Green’s function \( G_1(z) = (z-H_0-V_1^C)^{-1} \). The LSE (8) is the integral equation of the form

\[
\Psi^*(\mathbf{X}, \mathbf{p}_1) = \Phi_1(\mathbf{X}, \mathbf{p}_1) + \int d\mathbf{X}' G_1(\mathbf{X}, \mathbf{X}', E^+) [V_2^C(\mathbf{x}'_2) + V_3^C(\mathbf{x}'_3) + i g W_2(\mathbf{x}'_2)]\Psi^*(\mathbf{X}', \mathbf{p}_1),
\]

(10)

where \( \mathbf{X} = \{\mathbf{x}_1, y_1\} \) and \( \mathbf{x}'_j, \mathbf{y}'_j \) are supposed to be represented through \( \mathbf{x}_j, \mathbf{y}_j \), respectively, by standard transformations of Jacobi coordinates. The asymptotics of \( \Psi^*(\mathbf{X}, \mathbf{p}_1) \) as \( y_1 \to \infty \) can easily be evaluated from (10) by taking the asymptotics of Green’s function

\[
G_1(\mathbf{X}, \mathbf{X}', E^+) \propto \frac{-v_1}{2\pi \hbar^2} \phi_1(\mathbf{x}_1) e^{i \Phi_1} \Phi_1^*(\mathbf{X}', \sqrt{E - \epsilon_2 \hat{y}_1}).
\]

(11)

As a result, we get (7) with the following expression for the amplitude \( F \):

\[
F(\mathbf{p}_1^0, \mathbf{p}_1) = \frac{-v_1}{2\pi \hbar^2} \langle \Phi_1(\mathbf{p}_1^0) | V_2^C + V_3^C + i g W_2 | \Psi^*(\mathbf{p}_1) \rangle,
\]

(12)

where the matrix element stands for the integral

\[
\langle \Phi_1(\mathbf{p}_1^0) | V_2^C + V_3^C + i g W_2 | \Psi^*(\mathbf{p}_1) \rangle = \int d\mathbf{X}' \Phi_1^*(\mathbf{X}', \mathbf{p}_1^0) [V_2^C(\mathbf{x}'_2) + V_3^C(\mathbf{x}'_3) + i g W_2(\mathbf{x}'_2)]\Psi^*(\mathbf{X}', \mathbf{p}_1).\]

(13)

Formula (12) suggests that the scattering amplitude can be split into the sum of two terms

\[
F = F^0 + i g F^1,
\]

(14)

where \( F^0 \) is due to the Coulomb interactions between the positron and the hydrogen and \( F^1 \) is due to the absorption potential only. Let us note that the immediate identification of these amplitudes with pieces of (12) does not lead to the consistent form of the amplitudes \( F^k \) since the wavefunction \( \Psi^* \) itself may be split into two parts similar to (14). Hence, the contribution from different kinds of interactions cannot be separated on the basis of equation (12). The appropriate way is to rewrite the LSE (8) in the form of the distorted wave representation [14]. To this end, let us recast (8) into

\[
[I - G_1(E^+)(V_2^C + V_3^C)]\Psi^*(\mathbf{p}_1) = \Phi_1 + G_1(E^+)i g W_2 \Psi^*(\mathbf{p}_1).
\]

(15)

If the energy is below the positronium formation threshold, the inversion of the operator from the left-hand side can be performed with the help of the formulae

\[
[I - G_1(E^+)(V_2^C + V_3^C)]^{-1} \Phi_1 = \Psi^{0*},
\]

(16)

\[
[I - G_1(z)(V_2^C + V_3^C)]^{-1} G_1(z) = G^C(z),
\]

(17)

where \( G^C(z) = (z-H^C)^{-1} \). As a result, the LSE (8) takes the form

\[
\Psi^*(\mathbf{p}_1) = \Psi^{0*}(\mathbf{p}_1) + G^C(E^+)i g W_2 \Psi^*(\mathbf{p}_1).
\]

(18)
The asymptotic analysis of equation (18) will give us the representations for amplitudes $F^0$ and $F^1$.

The inhomogeneous term $\Psi^{0*}(p_1)$ is the outgoing solution to the $e^-\text{–H}$ scattering problem without the absorption potential. Following (16), this function is defined by the solution of the LSE

$$\Psi^{0*}(p_1) = \Phi_1(p_1) + G_1(E^*)(V_2^C + V_3^C)\Psi^{0*}(p_1).$$

(19)

Similar to (8), the asymptotics of the solution has the form

$$\Psi^{0*}(p_1) \propto \phi_1(x_1) \left[ e^{i\rho \cdot \tau_1} \frac{G_1(p_1)}{\gamma_1} F^0(p_1, p_1) \right]$$

(20)

with the amplitude given by

$$F^0(p_1', p_1) = \frac{-v_1}{2\pi \hbar^2} (\Phi_1(p_1') V_2^C + V_3^C |\Psi^{0*}(p_1))$$

(21)

Green’s function $G^C(z)$ asymptotics as $\gamma_1 \to \infty$ reads

$$G^C(x, x', E^*) \propto \frac{-v_1}{2\pi \hbar^2} \phi_1(x_1) \frac{e^{i\rho \cdot \gamma_1}}{\gamma_1} \Psi^{0*}(x', \sqrt{E - \epsilon_1})$$

(22)

Introducing this asymptotics into (18), we get the explicit representation for the amplitude $F^1$ from (14):

$$F^1(p_1', p_1) = \frac{-v_1}{2\pi \hbar^2} (\Psi^{0*}(p_1') W_2 |\Psi^*(p_1))$$

(23)

In these formulae, $\Psi^{0*}(p_1)$ is the solution of the $e^-\text{–H}$ scattering problem with incoming boundary conditions $\Psi^{0*}(p_1) \propto [\Psi^{0*}(-p_1)]^*$ when only Coulomb interactions are taken into account in the Hamiltonian. Formulae (21) and (23) provide us with the desired representation for $F$ as the sum of two amplitudes, one of which ($F^0$) is exclusively due to the Coulomb interactions between the positron and the hydrogen and does not depend on the absorption potential and the other one ($F^1$) is due to the absorption potential only.

The preceding analysis is not applicable if the energy $E$ is higher than the positronium formation threshold. Indeed, whereas formulae (6)–(14) remain valid, the inversion of the operator $I - G_1(E^*)(V_2^C + V_3^C)$ on the left-hand side of (15) cannot be performed, and therefore equations (18)–(23) cannot be justified. The formal reason is that the homogeneous equation

$$\chi = G_1(E^*)(V_2^C + V_3^C)\chi$$

(24)

possesses now the nontrivial solution $\chi = \Psi^{02}(p_2)$ such that

$$(H^C - E)\Psi^{02}(p_2) = 0$$

(25)

with the asymptotics $\Psi^{02}(p_2) \propto \phi_2(x_2) e^{i\rho \cdot \gamma_2}$. The latter describes the scattering of the proton off the positronium ground state $\phi_2(x_2)$ with the binding energy $\epsilon_2$.

This problem with LSE is well known in the three-body scattering theory [15–17] and is the manifestation of the general fact that no single LSE specifies the three-body scattering wavefunction uniquely, if the rearrangement channel is open. The resolution of the problem has been found by transforming LSE into the matrix equations for the components of the wavefunction. A proper arrangement of the interactions between the equations, which guarantees the uniqueness of the solution, leads to the equations known as the Faddeev three-body equations [16–19]. We apply this formalism to our case in the following subsection.
2.2. Three-body scattering formalism above the positronium formation threshold

Let us emphasize that the scattering problem with the Hamiltonian (1) always deals with the single-arrangement channel $e^+ - H$ due to the presence of an absorption potential. Therefore, the solution to the Schrödinger equation (6) has the single-arrangement asymptotics (7) irrespective of the energy which can be below or above the Ps-formation threshold. However, in order to specify the amplitudes $F^0$ and $F^1$ one needs the solutions to SE with the Hamiltonian $H^C$. For the energy above the Ps-formation threshold between $\text{Ps}(n = 1)$ and $H(n = 2)$ thresholds, the Schrödinger equation

$$H^C \Psi^0 = E \Psi^0$$

has two kinds of solutions, which are specified by the asymptotics

$$\Psi^0(p_i) \propto \phi_i(x_i) \left[ e^{ip_i y_i} + \frac{e^{ip_i y_i}}{y_i} f_{ii} \right], \quad y_i \to \infty,$$  \hspace{1cm} (27)

$$\Psi^0(p_i) \propto \phi_k(x_k) e^{ip_k y_k} f_{ki}, \quad y_k \to \infty, \quad k \neq i.$$  \hspace{1cm} (28)

Here the momenta $p_{i(k)}$ are related to the energy as

$$E = \frac{\hbar^2}{2m} \left( \frac{1}{v^2} \nu_i \nu_k \right) p_i^2 + \epsilon_i.$$  \hspace{1cm} (29)

Formulae (27) and (28) reflect the fact that now the asymptotic form of the wavefunction is different in different asymptotic arrangements. This is that property of the three-body wavefunction which cannot be recovered by any single LSE.

In order to take into account the multichannel character of the scattering problem above the rearrangement threshold, we use the formalism of Faddeev equations \[18\]. Since the original formalism is developed for the short-range interaction, at the first stage we reformulate the three-body Hamiltonian in such a way that Coulomb interactions are split into long-range and short-range parts \[19, 20\]:

$$V^C_i(x_i) = V^l_i(x_i, y_i) + V^s_i(x_i, y_i).$$

This splitting is made in the three-body configuration space by a smooth splitting function $\zeta_i(x_i, y_i)$ constructed such that $\zeta_i(x_i, y_i) = 1$ if $x_i/x_0 < (1 + y_i/y_0)^v$ and $\zeta_i(x_i, y_i) = 0$ if $x_i/x_0 > (1 + y_i/y_0)^v$ for some $x_0 > 0, y_0 > 0$ and $0 < v < 1/2$. Parameters $x_0, y_0$ are needed to make the definition non-dimensional and theoretically can be taken arbitrary finite \[19, 20\].

In practical calculations, the choice of $x_0, y_0$ is dictated by the reaction volume. With such $\zeta_i$, the short- and long-range parts of the Coulomb potentials are defined as

$$V^l_i(x_i, y_i) = \zeta_i(x_i, y_i) V^C_i(x_i), \quad V^s_i(x_i, y_i) = V^C_i - V^l_i.$$  \hspace{1cm} (30)

The Hamiltonian (1) is then transformed into

$$H = H^l + V^l_1 + V^l_2 + i g W_2, \quad H^l = T + V^l_1 + V^l_2 + V^C_3.$$  \hspace{1cm} (31)

After this modification, the components of the wavefunction $\Psi^+$ are defined by formulae

$$\Psi'^1 = (E^+ - H^l)^{-1} V^l_1 \Psi^+, \quad \Psi'^2 = (E^+ - H^l)^{-1} \left( V^l_2 + i g W_2 \right) \Psi^+.$$  \hspace{1cm} (32)

where $E^+ = E + i 0$. Two components are enough in our case. Indeed, the potential $V^C_3$ between the positron and the proton is repulsive and does not support bound states. Hence, only two asymptotic arrangements are possible, which are covered by components $\Psi'^{1,2}$.

It is straightforward to see that the sum of the components recovers the wavefunction

$$\Psi^+ = \Psi'^1 + \Psi'^2.$$  \hspace{1cm} (33)
and the components obey the set of modified Faddeev equations (MFE)

\[
\begin{align*}
(E - H^l - V^l_1)\Psi^+_1 &= V^+_1\Psi^+_1, \\
(E - H^l - V^l_2 - igW_2)\Psi^+_2 &= (V^+_2 + igW_2)\Psi^+_1.
\end{align*}
\]

The important feature of equations (32) and (33), with regard to the description of annihilation, is that the two-body absorption potential \(i gW_2\) is incorporated into equations in two manners. It appears in the diagonal part on the left-hand side of equation (33) and in the coupling term on the right-hand side. The diagonal terms of equations (32) and (33) are responsible for the asymptotic configurations in channels 1 and 2, so the absorption potential on the left-hand side of (33) is natural to associate with the annihilation after the positronium formation. The coupling term in (32) and (33) couples equations in the reaction volume; therefore the absorption potential on the right-hand side of (33) is the source for the direct annihilation process. These associations will be put on the solid ground in the following section.

As in the case of equation (6), the scattering solution to equations (32) and (33) is defined by the asymptotics as \(y_1 \to \infty\)

\[
\begin{align*}
\Psi^+_1(p_1) &\propto \phi_1(x_1) \left[ e^{ip_1y_1} + \frac{e^{ip_1\gamma_1}}{y_1} f_{11} \right], \\
\Psi^+_2(p_1) &\propto 0.
\end{align*}
\]

For the amplitudes \(F_{11}\) and \(F\) from (12), the equality holds true

\[ F_{11} = F \]

as it should be in view of (31). Similar to the case of equation (6), the solution required by (34) and (35) is given by the integral form of MFE (32) and (33) (IMFE), respectively,

\[
\begin{align*}
\Psi^+_1(p_1) &= \Phi^{0+}_1(p_1) + (E^+ - H^l - V^l_1)^{-1} V^+_1\Psi^+_2(p_1), \\
\Psi^+_2(p_1) &= (E^+ - H^l - V^l_2 - igW_2)^{-1} (V^+_2 + igW_2)\Psi^+_1(p_1).
\end{align*}
\]

Here \(\Phi^{0+}_1\) stands for the solution to the channel Schrödinger equation \((H^l + V^l_1 - E)\Phi^{0+}_1 = 0\), whose explicit form is

\[
(H_0 + V^C_1 - E)\Phi^{0+}_1 = -(V^+_2 + V^C_2)\Phi^{0+}_1.
\]

Repeating the reasoning of (8)–(13), we get the asymptotics as \(y_1 \to \infty\)

\[
\Phi^{0+}_1(p_1) \propto \Phi_1(p_1) + \phi_1(x_1) \frac{e^{ip_1\gamma_1}}{y_1} f_{11}^0
\]

with

\[
f_{11}^0(P_1, p_1) = \frac{-\gamma_1}{2\pi\hbar^2} \langle \Phi_1(p_1)|V^+_2 + V^C_2|\Phi_1^0(p_1)\rangle.
\]

The IMFE (36) and (37) are proven to have the unique solution below as well as above the rearrangement threshold \([18, 20]\). We use this property to remedy the above-outlined shortcoming of the LSE approach in specifying the structure of the amplitude \(F\) above the Ps-formation threshold.

In order to proceed, it is convenient to introduce matrix notations

\[
H(ig) = \begin{bmatrix}
H^l + V^l_1 & 0 \\
0 & H^l + V^l_2 + igW_2
\end{bmatrix}.
\]
Thus, the MFE set takes the form

$$[H(ig) - EI]\Psi(p_1) = -[V + igW]\Psi(p_1),$$  

(41)

where the vector solution is constructed from wavefunction components as \( \Psi = (\Psi_1^0, \Psi_2^0) \). The IMFE set (36) and (37) in matrix notations reads

$$\Psi(p_1) = \Phi^{0r}(p_1) + [E^*I - H(ig)]^{-1}[V + igW]\Psi(p_1).$$  

(42)

The vector of the inhomogeneous term is defined as \( \Phi^{0r}(p_1) = (\Phi_1^{0r}, 0) \). This equation can be reformulated in the form of the distorted wave representation by a similar way we made for LSE (8). Equation (42) can be recast into

$$[I - [E^*I - H(ig)]^{-1}V]\Psi(p_1) = \Phi^{0r}(p_1) + [E^*I - H(ig)]^{-1}igW\Psi(p_1).$$  

Then, by the use of the formulae

$$[I - [E^*I - H(ig)]^{-1}V]^{-1}\Phi^{0r}(p_1) = \Phi^{0r}(p_1),$$  

(43)

$$[I - [zI - H(ig)]^{-1}V]^{-1}[zI - H(ig)]^{-1} = [zI - H(ig) - V]^{-1},$$  

(44)

we arrive at the distorted wave representation of the IMFE

$$\Psi(p_1) = \Phi^{0r}(p_1) + [E^*I - H(ig) - V]^{-1}igW\Psi(p_1).$$  

(45)

From this equation, it is seen that

$$\Psi(p_1) = \Phi^{0r}(p_1) + \Phi^{1*}(p_1),$$  

(46)

where \( \Phi^{1*}(p_1) \) stands for the second term in equation (45). Equation (45) is the direct analogue of (18) but, in contrast to that, is well-defined below as well as above the Ps-formation threshold and therefore can be used to get the necessary representation for the amplitude \( F^0 \). The asymptotics of \( \Psi(p_1) \) is formed from contributions of both terms in (46). Let us first consider the inhomogeneous term \( \Psi^{0r}(p_1) \). The equation for this term reads

$$\Psi^{0r}(p_1) = \Phi^{0r}(p_1) + [E^*I - H(ig)]^{-1}V\Phi^{0r}(p_1)$$  

(47)

or

$$[H(ig) + V]\Psi^{0r}(p_1) = EI\Phi^{0r}(p_1).$$  

(48)

These equations are quite similar to (32), (33) and (36), (37) except for the coupling term \( V \), which does not contain the absorption potential. The asymptotics of the solution to (48) as \( y_1 \to \infty \), which follows from (47), is similar to (34) and (35) and for the components of \( \Psi^{0r} = (\Psi_1^{0r}, \Psi_2^{0r}) \) has the form

$$\Psi_1^{0r}(p_1) \propto \phi_1(x_1) \left[ e^{ip_1y_1} + \frac{e^{ip_1y_1}}{y_1} - F^0_{11} \right]$$  

(49)

$$\Psi_2^{0r}(p_1) \propto 0.$$  

(50)

The expression for the amplitude \( F^0_{11} \) should be derived by taking asymptotics of the right-hand side of (47) as \( y_1 \to \infty \). A minor difference from what we have demonstrated above is that the nontrivial contribution into the amplitude comes from not only Green’s function source term, but also from the driving term due to (39) so that the amplitude \( F^0_{11} \) is given by

$$F^0_{11}(p_1', p_1) = \frac{-\nu_1}{2\pi\hbar} [\langle \Phi_1(p_1')|V_2^2 + V_3^2|\Phi_1^{0r}(p_1)\rangle + \langle \Phi_1^{0r}(p_1')|V_1^1|\Psi_2^{0r}(p_1)\rangle].$$  

(51)
Now let us consider the $\Psi_{1+}^{\dagger}(p_1)$ term. Its asymptotics as $y_1 \to \infty$ is defined by Green's function $G(z) = [zI - H(ig) - V]^{-1}$. This function is a genuine three-body quantity and the asymptotics of its matrix elements as $y_2 \to \infty$ may be written in the form

$$G_{ij}(X, X', E^+) \propto \frac{-v_j}{2\pi \hbar} \phi_i(x_i) e^{ip_j y_j} \Upsilon_{j-i}^{0-}(X', \sqrt{E - \epsilon_j y_j}),$$

(52)

where $\Upsilon_{j-i}^{0-}$ is the eigenfunction of the adjoint to the operator from the left-hand side of (48). This asymptotics has a different character for $i = 1$ and $i = 2$. In the first case, $G_{1j}$ does not vanish with $y_j$ large since $E - \epsilon_j$ is real non-negative. If $i = 2$, the positronium binding energy $\epsilon_2$ becomes complex when the absorption potential is introduced into the $e^+e^-$ Hamiltonian. That makes the relative momentum $p_2 = \sqrt{2\nu_2/\hbar^2(E - \epsilon_2)}$ complex, i.e. $p_2 = p_2' + ip_2''$. So, the asymptotics of $G_{2j}$ vanishes exponentially as $\sim e^{-p'_2 y_j}$. Thus, only $\Psi_{1+}^{\dagger}$ component has the nontrivial asymptotics

$$\Psi_{1+}^{\dagger}(p_1) \propto \phi_1(x_i) e^{ip_j y_j} g F_{11}^1$$

(53)

with the amplitude $F_{11}^1$ given by

$$F_{11}^1(p_1, p_1) = \frac{-v_1}{2\pi \hbar} (\Upsilon_{2-}^{0+}(p_1) | W_2 | \Psi_1^0(p_1)).$$

(54)

Here $\Upsilon_{2-}^{0-}$ is the second component of the solution to the adjoint equation to (48)

$$[H(-ig) + V^T - E] \Upsilon_{2-}^{0-}(p_1) = 0.$$  

(55)

It is defined by the integral equation

$$\Upsilon_{2-}^{0-}(p_1) = \Phi_{2-}^{0-}(p_1) + [E^+ - H(-ig)]^{-1} V^T \Upsilon_{2-}^{0-}(p_1).$$

(56)

In this equation $E^+ = E - i0$, $V^T$ means the transposed matrix and $\Phi_{2-}^{0-} = (\Phi_{2-}^{0+}, 0)$ where $\Phi_{2-}^{0+}$ is the solution to (38) with incoming boundary conditions. The solution to (55) in the case of $g = 0$ takes the very simple form, i.e. $\Upsilon_{2-}^{0-} = \Upsilon_{2}^{0-} = \Psi^0$ where $\Psi^0$ is the three-body wavefunction for the pure Coulomb problem. So, $\Psi^0$ obeys the Schrödinger equation (26) and can be constructed from wavefunction Faddeev components (29) and (30) at $g = 0$ as $\Psi^0 = \Psi_{1+}^{0+} + \Psi_{2-}^{0+}$. The detailed information on this and other features of the matrix equations as MFE and IMFE and matrix Green’s functions, which is necessary for evaluations made above, can be found in [21].

Formulae (51) and (54) determine the ingredients of the amplitude $F_{11}^1$ uniformly above as well as below the rearrangement threshold of the positronium formation. It is possible to show by preforming backward transformations that below the Ps-formation threshold, where the representations (14), (21) and (23) are valid, the equality

$$F_{11}^0 + ig F_{11}^1 = F^{0+} + ig F^1 = F$$

(57)

holds true. It is important to note, that from the analysis of equation (47), it follows

$$F_{11}^0 = F^{0+} + O(g).$$

(58)

This means that the respective terms on the left- and right-hand sides of the first equation in the chain (57) are not identical. In fact the amplitude $F_{11}^1$ takes into account not only the Coulomb interaction between the positron and the hydrogen, as $F^{0+}$ does, but also the possibility of the $e^+e^-$ annihilation after the positronium formation. That is due to the presence of the absorption potential in the diagonal part of equation (48).
3. Optical theorem in the presence of absorption and annihilation cross section

3.1. Optical theorem

The standard optical theorem for Hermitian Hamiltonians is nothing but the manifestation of the flux conservation, what is equivalent to the unitarity of the S-matrix. The absorption potential breaks the Hermiticity and makes scattering not unitary. The lack of unitarity is the measure of how much of the flux is absorbed and in the case of annihilation is the way to determine the annihilation cross section. There is the extensive literature on the optical theorem, but [14] is the most suitable for our purpose. Following this approach by multiplying the SE (6) by complex conjugate wavefunction theorem, but [14] is the most suitable for our purpose. Following this approach by multiplying

\[ \Psi^* H_0 \Psi^* - \Psi^* H_0 \Psi^* = -2ig W_2 |\Psi^*|^2. \] (59)

Integrating over the domain \( \Omega_R = \{ \gamma_1 \leq R \} \), using Green’s formula and taking the limit as \( R \to \infty \), we get the following result:

\[ -2ig \int d\mathbf{x}_1 d\mathbf{y}_1 W_2 |\Psi^*|^2 = \frac{\hbar^2}{2\nu_1} \lim_{R \to \infty} \int R^2 d\mathbf{y}_1 \int d\mathbf{x}_1 \{\Psi^*, \Psi^*\}, \] (60)

which represents the balance of the flux. Here, the Wronskian \( \{\Psi^*, \Psi^*\} = \Psi^* \partial_y \Psi^* - \Psi^* \partial_y \Psi^* \) has to be taken under the condition \( \gamma_1 = R \). Then, using the asymptotic form of \( \Psi^* \) given in (7), the normalization of the ground-state wavefunctions \( \phi_1(\mathbf{x}_1) \) and the weak asymptotics of the plain wave (see, for example, [22])

\[ e^{\Psi y} \propto \frac{2\pi}{i\rho_y} [\overleftarrow{\delta} (\mathbf{p} - \mathbf{y}) e^{-i\rho_y} + \delta (\mathbf{p} - \mathbf{y}) e^{i\rho_y}], \]

we finally arrive at the optical theorem in the presence of absorption

\[ \frac{2\nu_1 (-g)}{\hbar^2 \rho_1} \int d\mathbf{x}_1 d\mathbf{y}_1 W_2 |\Psi^*|^2 = \frac{4\pi}{\rho_1} \text{Im} \, F(p_1, p_1) - \int d\mathbf{y}_1 \text{Im} \, F(p_1, \mathbf{y}_1, p_1)|^2. \] (61)

The positive quantity on the left-hand side of (61) is the absorption cross section which determines in our case the overall \( e^+ e^- \) annihilation cross section due to the direct process as well as due to annihilation after (virtual if \( E < \varepsilon_2 \) or actual if \( E > \varepsilon_2 \)) positronium formation

\[ \sigma^a = \frac{2\nu_1 (-g)}{\hbar^2 \rho_1} \int d\mathbf{x}_1 d\mathbf{y}_1 W_2 |\Psi^*|^2, \] (62)

so that the overall annihilation cross section can be computed either by the integral (62) or by the expression on the right-hand side of (61), if the total amplitude \( F \) is in possession.

In order to go beyond the standard formulation (61) and (62), one needs to use the detailed structure of the amplitude \( F \). In our case, it is the representation (57)

\[ F = F_{11}^0 + ig F_{11}^1, \]

which leads to the following form of (61):

\[ \sigma^a = \sigma^a_2 + \sigma^a_1 \] (63)

\[ \sigma^a_2 = \frac{4\pi}{\rho_1} \text{Im} \, F_{11}^0 (p_1, p_1) - \int d\mathbf{y}_1 \text{Im} \, |F_{11}^0 (p_1, \mathbf{y}_1, p_1)|^2 \] (64)

\[ \sigma^a_1 = \frac{4\pi}{\rho_1} (-g) \text{Re} \, F_{11}^1 (p_1, p_1) - 2(-g) \int d\mathbf{y}_1 \text{Im} \, F_{11}^0 (p_1, \mathbf{y}_1, p_1) F_{11}^1^{*} (p_1, \mathbf{y}_1, p_1) \]

\[ -g^2 \int d\mathbf{y}_1 |F_{11}^1 (p_1, \mathbf{y}_1, p_1)|^2. \] (65)
The quantities $\sigma_1^a$ and $\sigma_2^a$ have a meaning of annihilation cross sections for the direct process and the process of annihilation after the positronium formation. To make this statement sound, let us show that $\sigma_2^a$ is the cross section of annihilation after the positronium formation. Thus, the remaining part of $\sigma^a$, what is $\sigma_1^a$, should be interpreted as the direct annihilation cross section.

It is apparent that equation (64) is the optical theorem formulated for equation (48). Indeed, multiplying equation (48) by $\Psi^{0*}$ from the right and making obvious cancellations, we get

$$\langle \Psi^{0*}, H_0 \Psi^{0*} \rangle - \langle H_0 \Psi^{0*}, \Psi^{0*} \rangle = -2i g \langle \Psi^{0*}, D \Psi^{0*} \rangle.$$  

Here, $D$ is the diagonal matrix $\text{diag}[0, W_2]$ and $(\cdot, \cdot)$ is the inner product in the two-dimensional complex space $\mathbb{C}^2$ of wavefunction components. Repeating arguments which led us to formula (61), we arrive at the equality

$$\frac{2v_1 (g)}{\hbar^2 p_1} \int dx_1 dy_1 \Upsilon_2^{0*}(p_1) W_2 \Psi_2^{0*}(p_1) = \frac{4\pi}{p_1} \text{Im} F_{11}^0(p_1, p_1) - \int d\gamma |F_{11}(p_1, \gamma, p_1)|^2.$$  

This is the optical theorem for equation (48) and the annihilation cross section $\sigma_2^a$ can be expressed now in terms of the left-hand side as

$$\sigma_2^a = \frac{2v_1 (g)}{\hbar^2 p_1} \int dx_1 dy_1 \Upsilon_2^{0*}(p_1) W_2 \Psi_2^{0*}(p_1).$$  

To elucidate the further meaning of the cross section $\sigma_2^a$, it is instructive to consider the limiting case as $g \to 0$. In the limit no absorption potential is present, scattering becomes unitary and amplitude $F_{11}^0$ coincides with $f_{11}$ from (27). The standard unitary variant of the optical theorem for the amplitude $f_{11}$ has the form

$$\frac{4\pi}{p_1} \text{Im} f_{11}(p_1, p_1) - \int d\gamma |f_{11}(p_1, \gamma, p_1)|^2 - \int d\gamma |f_{21}(p_1, \gamma, p_1)|^2 = 0$$  

where $f_{11}$ is the elastic $e^+ - H$ amplitude and $f_{21}$ is the rearrangement Ps--$p$ amplitude. Therefore, the right-hand side of (67) has the limit

$$\frac{4\pi}{p_1} \text{Im} F_{11}^0(p_1, p_1) - \int d\gamma |F_{11}^0(p_1, \gamma, p_1)|^2 \to \int d\gamma |f_{21}(p_1, \gamma, p_1)|^2 = \sigma_{21}.$$  

The quantity $\sigma_{21}$ is nothing but the positronium formation cross section. At the same time, formula (68) leads to an uncertainty in the limit as $g \to 0$ when the diverging integral is multiplied by the vanishing factor $g$. The resolution of this uncertainty is made by (70) and gives the relation

$$\sigma_2^a = \sigma_{21} + O(g),$$

which clearly shows that $\sigma_2^a$ is the cross section of annihilation after the positronium formation.

The main result of this subsection is the representation of the annihilation cross section as the sum of two terms

$$\sigma^a = \sigma_1^a + \sigma_2^a,$$

where $\sigma_2^a$ is shown to represent the cross section of annihilation after the positronium formation, which is given by formula (64) or (68). Therefore $\sigma_1^a$ is the direct annihilation cross section, given by (65).

The analysis made above shows that the definitions of cross sections in terms of scattering amplitudes (64) and (65) are uniform and are valid below as well as above the rearrangement
threshold of the positronium formation. Moreover, by construction, the integrals (51) and (54) involved in the definitions of the amplitudes $F_{11}^0$, $F_{11}^1$ have finite limits as $g \to 0$. This property will be used below for perturbative calculations of the amplitudes and cross sections. At the same time, the integrals in representations (62) and (68) are divergent above the positronium formation threshold if the limit $g \to 0$ is taken. That makes these formulae not suitable for perturbative methods above the positronium formation threshold.

3.2. Absorbing annihilation potential

In this subsection we fix the coordinate form of the absorption potential by comparing the definition (62) for $\sigma^a$ with the perturbative QED formula for the $2\gamma$ singlet $e^+e^-$ annihilation\footnote{The spin-averaging factor 1/4 for the singlet $2\gamma$ annihilation is implied implicitly.} [2, 3]

$$\sigma^a = \pi r_0^2 (c/v) Z_{\text{eff}}.$$  (72)

In this formula $r_0$ is the classical electron radius, $c$ is the speed of light and $v$ is the incident velocity of the positron. The effective number of electrons $Z_{\text{eff}}$ participating in the annihilation is given by the integral

$$Z_{\text{eff}} = \int d x_1 \, d y_1 |\Psi_0^{\text{inc}}(x_1, y_1)|^2 \delta(x_2).$$  (73)

Here $\Psi_0^{\text{inc}}$ is identical to the $\Psi_0$ solution of the $e^+-H$ scattering problem (26)–(28) when the absorption potential is not taken into account. The integral in (73) is well defined below the Ps-formation threshold. In this case (72) and (73) can be considered as the first-order perturbation approximation to the exact absorption cross section (62), since below the rearrangement threshold $\Psi_0^{\text{inc}} \approx \Psi_0^{\text{inc}}$ is the well defined first-order perturbation solution (Born) to (18). This observation was used in [4] to determine the absorption potential for $2\gamma$ singlet $e^+e^-$ annihilation as

$$i g W_2(x_2) = i g \delta(x_2) \quad g = -\frac{e^2}{a_0^2} 2 \pi \alpha^3.$$  (74)

Here $a_0$ is the Bohr radius and $\alpha$ is the fine structure constant. This potential was used in [4] to calculate the direct annihilation cross section by solving the Lippmann–Schwinger equation for T-matrix below the Ps-formation threshold.

Formula (73) cannot be extended for calculations above the Ps-formation threshold since the integral diverges. One of the ways to go over the Ps-formation threshold is the use of (62) with the absorption potential (74) incorporated into the Schrödinger equation. This was done in [5, 7] where the overall annihilation cross section $\sigma^a$ was computed below as well as above the Ps-formation threshold within the hyperspherical close coupling technique for the time-independent three-body Schrödinger equation. Yamanaka et al [8] represent the solution of the time-dependent three-body Schrödinger equation with the absorption potential (74) below as well as above the Ps-formation threshold. All these papers dealt with numerical solutions of respective equations, and the delta-functional singularity of the potential (74) was treated by a certain numerical approximation. Nevertheless, the analytical status of the potential (74) is not satisfactory. The delta-functional singularity is too strong and makes the Hamiltonian not well defined. This issue was not addressed in aforementioned papers, and we give a portion of the necessary analysis in this subsection.

It is well known already since the papers by Fermi [9] and then Breit [10] that the three-dimensional delta-function potential can be incorporated into the Schrödinger equation only perturbatively. One of the approaches to go beyond the perturbative treatment is the use of
a zero-range potential [10, 11]. There are two common ways to introduce the zero-range potential. One is imposing boundary conditions for the wavefunction at the singularity point. The other one is introducing an additional term into the Hamiltonian, which enforces the wavefunction to fulfil the boundary conditions. This term can conveniently be represented in the compact form by the quasi-potential [23, 24]. We follow the second option.

The singularity caused by the zero-range potential in the case of the electron–positron interaction is located at the same point as the Coulomb singularity $-e^2/x_2$. The latter leads to the modification of the standard zero-range potential and of the respective quasi-potential [25]. The resulting form for the coordinate part $W_2$ of the absorption potential, which can in principle be derived by methods of [25], reads

$$W_2(x) = \delta(x) \frac{1 - n_2 x}{1 + n_2 x \log x} \frac{d}{dx} \frac{x}{1 + n_2 x \log x}, \quad (75)$$

where $n_2 = -2\mu_2 e^2$ and $\mu_2$ is the $e^+e^-$ reduced mass. The detailed derivation of (75) is out of the scope of this paper and will be published elsewhere. Some basic theorems about general properties of the zero-range potential with the Coulomb modification can be found in [26].

It is straightforward to see that in the limit $n_2 \to 0$, the quasi-potential (75) takes the usual form

$$W_2(x) \to \delta(x) \frac{d}{dx} x. \quad (76)$$

The quasi-potential $i\gamma W_2(x_2)$ enforces the following asymptotics for the wavefunction as $x_2 \to 0$

$$\Psi(x_2, y_2) \propto \frac{a(y_2)}{4\pi} \left[ \frac{1}{x_2} + n_2 \log x_2 \right] + b(y_2) + O(x_2 \log x_2), \quad (77)$$

where $a/b = -i\gamma 2\mu_2/\hbar^2$. This asymptotics determines the appropriate boundary conditions, which we do not write down here explicitly. The action of the quasi-potential (75) on the function with the asymptotics (77) is given by the formula

$$W_2(x_2)\Psi(x_2, y_2) = \delta(x_2)b(y_2). \quad (78)$$

The latter means that the action of the quasi-potential on a function $\chi(x_2, y_2)$, which is regular at $x_2 = 0$, is equivalent to the delta function

$$W_2(x_2)\chi(x_2, y_2) = \delta(x_2)\chi(0, y_2). \quad (79)$$

Therefore, if a matrix element of the quasi-potential (75) is calculated between the functions $\chi, \omega$, which are regular at $x_2 = 0$, then the quasi-potential is equivalent to the delta function, i.e.

$$\langle \chi | W_2(x_2) | \omega \rangle = \langle \chi | \delta(x_2) | \omega \rangle. \quad (80)$$

This statement justifies the use of the delta function as the coordinate part of the absorption potential in [5, 7, 8], since the basis functions of the approaches used to compute the matrix elements of the absorption potential are smooth. Nevertheless, any basis of smooth functions cannot reproduce the singularity in (77) by a finite number of terms, what always happens along the numerical solution. Hence, such a treatment of the zero-range potential in [5, 7, 8] is approximative but, in view of the fact $a(y_2) = -i\gamma 2\mu_2 b(y_2)/\hbar^2$ with $|\gamma| \ll 1$ for the $e^+e^-$ annihilation, the approximation is reasonable.
4. Calculation of the annihilation cross section

The formalism developed above was applied for calculations of the annihilation in $e^+\text{–H}$ collision below the Ps-formation threshold and above the threshold in the Ore gap. The latter is defined as the interval of the energy between the Ps($1s$) and H($n=2$) thresholds. All calculations were made on the basis of an extension of the multichannel numerical algorithm for Faddeev equations, described in details in [27], for the case of annihilation. The algorithm uses the bipolar harmonic expansion to represent the angular dependence of the wavefunction components

$$
\Psi_{L}^{s}(x_{i},y_{i}) = \sum_{gL,i_{L},i_{L}}^{} \frac{\psi_{g_{L},i_{L}}^{s}(x_{i},y_{i})}{x_{i}y_{i}} Y_{LM}^{L}(\hat{x}_{i},\hat{y}_{i}),
$$

(81)

This expansion reduces the MFE to a set of coupled equations for radial components $\psi_{g_{L},i_{L}}^{s}(x_{i},y_{i})$ which are then approximated by the quintic-spline expansion and solved by the orthogonal collocation procedure.

In order to test the numerical approach, the genuine Coulomb problem for $e^+\text{–H}$ scattering was solved on the platform of MFE (32) and (33) with $g=0$. The convergent result within the uncertainty less than 1% for s-wave phase shift $\delta_{0}$ was obtained with values of the relative momenta $l_{1}, l_{2}$ in expansion (81), ranging from 12 to 15 depending on the energy. The calculated s-wave phase shift recovers up to the three significant digits the results of previous Faddeev calculations [28] and the results of other calculations [29, 30, 34] in the diapason of the representation (65). The amplitudes $\sigma_{a_{1}}^{s}$ were computed from the solutions of the respective Faddeev equations. The effective number $Z_{\text{eff}}^{1}$ for the direct annihilation cross section was obtained using the expression similar to (72)

$$
\sigma_{a_{1}}^{s} = \pi r_{0}^{2} (c/v) Z_{\text{eff}}^{1},
$$

(82)

As was mentioned in subsection 3.1, calculating the amplitudes $F_{01}^{0}$ and $F_{11}^{1}$, we have systematically approximated the Faddeev components, involved in the matrix elements for the amplitudes, by the solutions $\psi_{f}^{0\pm}$ of the MFE with $g=0$. This approximation can easily be justified by the iterative solution of the IMFE (36) and (37) for $|g| \ll 1$. The iterative solutions is well defined, thanks to the fact that the matrix kernel of the Faddeev equation is proven to be compact. As a result, the expression for the absorption amplitude $F_{11}^{1}$ from (54) can be simplified as

$$
F_{11}^{1}(\mathbf{p}_{1}, \mathbf{p}) = \frac{-v_{1}}{2\pi\hbar^{2}} \langle \psi_{1}^{00}(\mathbf{p}_{1}) + \psi_{2}^{00}(\mathbf{p}_{1}) | W_{2} | \psi_{1}^{00s}(\mathbf{p}_{1}) \rangle,
$$

(83)

which was used for calculations of this paper.

In table 1 we display our calculated phase shift $\delta_{0}$ and $Z_{\text{eff}}^{1}$ together with results of other authors obtained with the standard formula (72) for one of the typical values of the relative momentum $p_{1} = 0.4 \ [1/a_0]$. The agreement is very good for calculations made by quite different approaches. In table 2 we collect the results of existing calculations of $Z_{\text{eff}}$ well below the Ps-formation threshold to compare with our results. One cannot expect a complete agreement since our definition of $\sigma_{a}^{s}$ concerns the direct process only, whereas the standard definition below the Ps-formation threshold deals with the overall annihilation cross section $\sigma_{a}$. However, if the indirect cross section $\sigma_{a}^{\sigma}$ is added to $\sigma_{a}^{s}$, then our results reproduce the results of previous Faddeev calculations [28]. It shows that the contribution of the indirect process does not exceed few per cents in the considered energy interval.
Figure 1. The effective number $Z_{\text{eff}}$ for the $L = 0$ direct annihilation. The diamonds are the calculations of the present paper (ZYH), the open squares (ZYK) are the data from [8], the triangle marks the positronium formation threshold.

Table 1. $L = 0$ phase shift $\delta_0$ for $e^+–H$ elastic scattering and effective number $Z_{\text{eff}}$ for the relative momentum $p_1 = 0.4 [a_0^{-1}]$.

| Reference | $\delta_0$ | $Z_{\text{eff}}$ |
|-----------|------------|-----------------|
| Present work | 0.119 83 | 3.3293 |
| [31]       | 0.119 8 | 3.232 |
| [29]       | 0.120 1 | 3.327 |
| [32]       | 0.119 8 | 3.407 |
| [33]       | 0.119 1 | 3.332 |

Table 2. $L = 0$ effective number $Z_{\text{eff}}$ for $e^+–H$ annihilation. The relative momenta $p_1$ are given in units of $a_0^{-1}$.

| $p_1$ | Present work | [28] | [34] | [35] |
|-------|--------------|------|------|------|
| 0.1   | 7.2570       | 7.55 | 7.5  | 7.363 |
| 0.2   | 5.1627       | 5.74 | 5.7  | 5.538 |
| 0.3   | 4.1061       | 4.36 | 4.3  | 4.184 |
| 0.4   | 3.3293       | 3.4  | 3.3  | 3.327 |
| 0.5   | 2.8118       | 2.74 | 2.7  | 2.73  |
| 0.6   | 2.4625       | 2.29 | 2.3  | 2.279 |
| 0.7   | 2.2529       | 2.02 |       | 1.950 |

The calculations of the direct annihilation cross section $\sigma_1^a$ were made in the interval of the energy between H($n = 1$) and H($n = 2$) thresholds on the basis of the formula (65). Figure 1 shows the s-wave effective number $Z_{\text{eff}}^s$ derived from $\sigma_1^a$ with formula (82) and results of calculations from [8]. Although, quite different methods (time-independent Faddeev equations and time-dependent wave-packet approach to the Schrödinger equation) of calculations for the direct annihilation cross sections have been used, the agreement between the data is fairly good. In fact, the definition of the direct cross section $\sigma_1^a$ in our formalism as the remainder of the overall annihilation cross section $\sigma^a$ after subtraction of the annihilation cross section after the Ps formation $\sigma_2^a$,

\[
\sigma_1^a = \sigma^a - \sigma_2^a,
\]  

(84)
Table 3. $L = 0$ effective number $Z_{\text{eff}}^1$, the direct annihilation cross section $\sigma_1^d$, and the positronium formation cross section $\sigma_{21}$. The cross sections are given in units of $\pi a_0^2$ and momenta in units of $a_0^{-1}$. The abbreviation $[\cdot n]$ is used for $10^{-n}$.

| $p_1$ | $Z_{\text{eff}}^1$ | $\sigma_1^d$ | $\sigma_{21}$ |
|-------|-------------------|--------------|--------------|
| 0.70654 | 2.3289 | 1.28 $[-6]$ | 9.05 $[-4]$ |
| 0.71 | 2.1715 | 1.19 $[-6]$ | 4.14 $[-3]$ |
| 0.8 | 1.8640 | 9.05 $[-7]$ | 5.03 $[-3]$ |
| 0.85 | 1.7404 | 7.95 $[-7]$ | 5.83 $[-3]$ |
| 0.861 | 1.4840 | 6.69 $[-7]$ | 0.01087 |
| 0.861 | 1.9678 | 8.88 $[-7]$ | 0.01682 |
| 0.861 | 2.2200 | 1.00 $[-6]$ | 0.02694 |
| 0.861 | 2.3022 | 1.04 $[-6]$ | 0.02943 |
| 0.861 | 2.4175 | 1.09 $[-6]$ | 0.03247 |
| 0.861 | 2.5832 | 1.16 $[-6]$ | 0.03622 |
| 0.861 | 2.7817 | 1.25 $[-6]$ | 0.04087 |
| 0.861 | 3.1700 | 1.43 $[-6]$ | 0.05380 |
| 0.861 | 0.9735 | 4.39 $[-7]$ | 0.07030 |
| 0.861 | 0.9742 | 4.39 $[-7]$ | 0.07450 |
| 0.861 | 1.4915 | 6.73 $[-7]$ | 0.02089 |
| 0.861 | 1.6459 | 7.42 $[-7]$ | 0.00013 |
| 0.861 | 1.7034 | 7.68 $[-7]$ | 0.00083 |
| 0.861 | 1.7674 | 7.97 $[-7]$ | 0.00326 |

Table 4. $L = 1$ effective number $Z_{\text{eff}}^1$, the direct annihilation cross section $\sigma_1^d$ and the positronium formation cross section $\sigma_{21}$. The cross sections are given in units of $\pi a_0^2$ and momenta in units of $a_0^{-1}$. The abbreviation $[\cdot n]$ is used for $10^{-n}$.

| $p_1$ | $Z_{\text{eff}}^1$ | $\sigma_1^d$ | $\sigma_{21}$ |
|-------|-------------------|--------------|--------------|
| 0.8 | 0.5404 | 2.62 $[-7]$ | 0.485 |
| 0.85 | 0.6933 | 3.17 $[-7]$ | 0.566 |
| 0.863 | 0.4775 | 2.15 $[-7]$ | 0.749 |
| 0.863 | 0.4695 | 2.11 $[-7]$ | 0.848 |
| 0.863 | 0.4675 | 2.10 $[-7]$ | 1.022 |
| 0.863 | 0.3914 | 2.66 $[-7]$ | 1.772 |
| 0.863 | 4.8319 | 2.17 $[-6]$ | 3.680 |
| 0.863 | 14.6255 | 6.58 $[-6]$ | 1.770 |
| 0.863 | 2.1967 | 9.88 $[-7]$ | 0.129 |
| 0.863 | 0.9012 | 4.06 $[-7]$ | 0.068 |
| 0.863 | 0.5629 | 2.53 $[-7]$ | 0.407 |

(see equation (63)) is to some extent similar to the time-dependent definition by formula (7) of [8]. Nevertheless, as the data of tables 3 and 4 show, the direct use of formula (84) would be very unpractical. The formation cross section $\sigma_{21}$, which is the leading term of $\sigma_a^d$ due to (71), rapidly increases above the threshold and is several orders of magnitude larger than $\sigma_a^d$. The analytic separation of the overall annihilation cross section into the formation and direct parts made in subsection 3.1 and given by formulae (63)–(65) in terms of amplitudes $F_{01}^1$ and $F_{11}^1$ is therefore of great practical importance.

In tables 3 and 4, we present the results of our calculations for the direct annihilation cross section together with the cross section of the positronium formation above the Ps-formation
threshold. They are given for slightly different values of momenta $p_1$ for $L = 0$ and $L = 1$ in order to emphasize the most characteristic behaviour of cross sections near the respective Feshbach resonances. Besides the expected difference in several orders of magnitude between the direct annihilation cross section $\sigma_1^a$ and the positronium formation cross section $\sigma_2^{t,h}$, the strong correlation between these cross sections in the region of the sharp increase of $\sigma_1^a$ across \(0.861 \, a_0^{-1}\) for $L = 0$ and $0.863 \, 18 \, a_0^{-1}$ for $L = 1$ is clearly seen. The graphical representation of that sharp increase of cross sections is given in figures 2 and 3 which display $s$- and $p$-wave $Z_{\text{eff}}$. This resonant feature was also observed in the spatial behaviour of the solution to the Faddeev equation. The first component $\Psi_1^s$, which is related to the $e^+–H$ channel, always exhibits the characteristic resonant bump near resonant energy. These spatial resonant structures can be extensive depending on the lifetime of the resonances. In [13], reasonable estimations of the energy width of a number of Feshbach resonances were made.
using the uncertainty principle applied to the graphical representation of the wavefunction components.

5. Conclusion

In the present paper, we have developed the multichannel time-independent formalism, which is capable of describing the scattering and annihilation processes in the positron–hydrogen collision above the rearrangement threshold. The expression derived in the paper for the direct annihilation cross section in terms of amplitudes is proven to extend the standard formula to the energy region above the positronium formation threshold. Below the threshold our cross section and the cross section calculated from the standard theory are in good agreement provided the close vicinity of the positronium formation threshold is not considered, where the cross section computed from the standard formula becomes infinite. The direct annihilation cross section defined by the formula (65) does not exhibit any singular behaviour at the Ps-formation threshold. It is in good agreement with the nonsingular direct annihilation cross section computed from the time-dependent solution of the three-body Schrödinger equation for the e⁺–H system [8].

The formalism of this paper can readily be extended beyond the Ore gap. In this case the multichannel optical theorem, which generalizes (61), plays the key role in the determination of cross sections. Preliminary calculations indicated the much larger enhancement of the direct annihilation cross section near the Feshbach resonances in the eight open channel region above the Ps\((n = 2)\) threshold. Since there are numerous resonances beyond the Ore gap, they evidently made a significant contribution to the overall annihilation peak around 12 eV displayed in figure 2 of [8]. We hope that our individual annihilation resonance structure will provide a new experimental tool to study sharp resonances. Although at the present time it is not possible to conduct such an experiment for the e⁺–H system, experiments for positron scattering on large molecules have been done for many systems [36].

Our approach, in perspective, opens the way to considering more complicated systems with more than three particles, as for example e⁺e⁺e−e−. Suitable formalism for multichannel scattering [37], which is the generalization of the Faddeev equations for the four-particle systems, will be helpful as an important theoretical step towards the experimental verification and utilization of the rich positron annihilation physics.

Acknowledgments

The authors appreciate the support of the NSF grant Phy-0243740, INTAS grant no. 03-51-4000 and the generous supercomputer time awards from grants MCA96T011 and TG-MCA96T011 under the NSF partnership for Advanced Computational Infrastructure, Distributed Terascale Facility (DTF) to the Extensible Terascale Facility. In particular we are thankful to PSC and SDSC. The authors would like to thank Dr Y Kino for providing us with numerical data corresponding to figure 2 of [8], which made the comparison of our results much feasible. We are grateful to Professor K A Makarov for fruitful discussions on zero-range potentials and Professor Z Papp for critical reading of the manuscript.

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