High resolution calculations of low energy scattering in \( e^- e^+ p^- \) and \( e^+ e^- He^{++} \) systems via Faddeev–Merkuriev equations

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Abstract

The potential splitting approach incorporated into the framework of Faddeev–Merkuriev equations in the differential form is used for calculations of multichannel scattering in \( e^- e^+ p^- \) and \( e^+ e^- He^{++} \) systems. Detailed calculations of all possible S-wave cross-sections are performed in the low-energy region which supports up to seven open channels including the rearrangement channels of ground and excited states of antihydrogen, positronium and helium ion formations. All known sharp resonances of the systems obtained and approved by a number of authors are clearly reproduced in the calculated cross sections. In cross sections for energies above the threshold corresponding to \( n = 2 \) state of antihydrogen the prominent oscillations of Gailitis–Damburg type have been found.

Keywords: Faddeev–Merkuriev equations, positron scattering, antihydrogen formation

(Some figures may appear in colour only in the online journal)

1. Introduction

Study of electron and positron scattering off light atomic targets (like (anti)hydrogen atom and helium cation) is of fundamental importance for atomic physics. These colliding systems represent genuine three-body Coulombic systems with variety of channels and with rich resonant structure of scattering cross sections. Many calculations have been performed by now for elastic and reactive scattering in these systems based on different computational platforms. Among others, the variational methods \([1–4]\), close coupling \([5, 6]\), hyperspherical close coupling \([7, 8]\) approaches and methods of Faddeev–Merkuriev (FM) equations \([9–13]\) are in extensive use. Another group of methods exploits complex rotation of coordinates \([14]\) and complex rotation with potential splitting \([15–20]\). The latter is especially designed to treat the asymptotic Coulomb interaction and have been successfully applied for elastic electron(positron)-hydrogen and electron (positron)-helium cation collisions.

Besides the features related to the long range character of the Coulomb interaction, collisions in \( e^- H, e^- H^+ \) and \( e^+ He^- \) systems also exhibit the fundamental rearrangement phenomenon of positronium (electron–positron bound state) formation. For such a case the solution methods should be capable of representing the solution for all the asymptotic fragmentations accurately. The Faddeev equations \([21]\) were designed especially to fulfill this requirement first for short-range interactions, and then a generalization for the long-range Coulomb case was developed by Merkuriev \([22]\). This generalization—called the FM equations—is based on the Coulomb potential splitting into the interior and the long range tail parts leading to the mathematically rigorous boundary value problem, which solution is strictly equivalent to the solution of the Schrödinger equation \([21]\). This approach suits the computationally difficult detailed low energy elastic and reactive scattering calculations in three-body Coulomb systems perfectly \([10, 11, 23]\). Typically, the splitting is being done by an artificial functional parameter in the three-body configuration space called the Merkuriev cut-off function. Recently, we showed that for low-energy collisions a much simpler splitting in two-body configuration

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space can be used [24]. In this contribution we present some basic guidelines for the choice of the cut-off function in the two-body configuration space, thus minimizing the number of free parameters of the splitting procedure. Following these guidelines allows us to produce more accurate results with smaller computational efforts. Additionally, a special numerical technique for handling the matrices, known as ‘tensor trick’, drastically reduces the computational complexity of the numerical solution of the FM equations [25, 26].

Here, the formalism of FM equations has been used to calculate S-wave cross sections in e−e+He++ systems in the low-energy region for all open channels. Even though there exist many calculations available in the literature, still there is some lack of high-precision and detailed results especially for the e−e+He++ system, which is one of the reasons for performing this research. Besides, a special emphasis is made on antihydrogen formation by antiproton impact of positronium which is currently used in experiments on antimatter at CERN (see [27] and references therein).

The paper is organized as follows. In section 2 we give the necessary portion of the three-body FM equations formalism with splitting of the long-range Coulomb potential. Section 3 describes the solution technique of the resulting FM equations in the total angular momentum representation in 3D configuration space. Section 4 contains results of calculations of low-energy reactive scattering in e−e+He++ systems. Last section 5 concludes the paper.

Throughout the paper we use atomic units.

2. Theory

We consider the system of three spinless nonrelativistic charged particles of masses \(m_\alpha\) and charges \(Z_\alpha, \alpha = 1, 2, 3\). In what follows the set of indices \(\{\alpha, \beta, \gamma\}\) runs over the set \(\{1, 2, 3\}\) enumerating particles and it is also used for identifying the complementary pair of particles, since in the partition \(\{\alpha(\beta\gamma)\}\) the pair of particles \(\beta\gamma\) is uniquely determined by the particle \(\alpha\). The standard Jacobi coordinates are defined for a pair \(\alpha(\beta\gamma)\) as relative position vectors between the particles of the pair \(\beta\gamma\) and between their center of mass and the particle \(\alpha\). In applications it is convenient to use reduced Jacobi coordinates \(x_\alpha, y_\alpha\), which are Jacobi vectors scaled by factors \(\sqrt{2}m_\alpha\) and \(\sqrt{2}m_\alpha\), respectively, where the reduced masses are given by

\[
\mu_\alpha = \frac{m_\beta m_\gamma}{m_\beta + m_\gamma}, \quad \mu_{\alpha(\beta\gamma)} = \frac{m_\alpha (m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma}.
\]

(1)

For different \(\alpha\)’s the reduced Jacobi vectors are related by an orthogonal transform

\[
x_\beta = c_{3\beta} x_\alpha + s_{3\beta} y_\alpha, \quad y_\beta = -s_{3\beta} x_\alpha + c_{3\beta} y_\alpha,
\]

(2)

where

\[
c_{3\beta} = \left( \frac{m_\beta m_\gamma}{(M - m_\beta)(M - m_\gamma)} \right)^{1/2},
\]

\[
s_{3\beta} = (-1)^{\beta - \alpha} \text{sgn}(\alpha - \beta)(1 - c_{3\beta}^2)^{1/2}
\]

\(M = \sum_\alpha m_\alpha\). In what follows where it is due, it is assumed that \(\beta\) Jacobi vectors are represented through \(\alpha\) vectors via (2).

In these reduced Jacobi coordinates FM equations for three charged particles [21] read

\[
\left\{ T_0 + V_\alpha(x_\alpha) + \sum_{\beta\neq\alpha} V^{(1)}_{\alpha\beta}(x_\beta, y_\beta) - E \right\} \psi_\alpha(x_\alpha, y_\alpha) = -V^{(1)}_{\alpha\beta}(x_\alpha, y_\alpha) \sum_{\beta\neq\alpha} \psi_\beta(x_\beta, y_\beta). \tag{3}
\]

Here \(T_0 \equiv -\Delta x_\alpha - \Delta y_\alpha\) are the kinetic energy operators. Throughout the paper the magnitude of a vector \(x\) is denoted by \(x\), i.e. \(x = |x|\), and \(\hat{x} = x/x\) stands for a unit vector. The potentials \(V_\alpha\) represent the pairwise Coulomb interaction \(V_\alpha(x_\alpha) = 2\mu_\alpha Z_\beta Z_\gamma /|x_\alpha| (\beta, \gamma \neq \alpha)\), although a short-range (decreasing as \(1/|x_\alpha|^2\) or faster as \(x_\alpha \to \infty\)) potential can also be included in the formalism. Throughout the paper we assume \(Z_\beta Z_\gamma > 0, Z_\beta Z_\gamma < 0\) and \(Z_\beta Z_\gamma < 0\) hold, thus \(V_\alpha\) is always repulsive. The potentials \(V_\alpha\) are split into the interior (short-range) \(V^{(s)}_\alpha\) and the tail (long-range) parts \(V^{(l)}_\alpha\)

\[
V_\alpha(x_\alpha) = V^{(s)}_\alpha(x_\alpha, y_\alpha) + V^{(l)}_\alpha(x_\alpha, y_\alpha). \tag{4}
\]

The equation (3) can be summed up leading to the Schrödinger equation for the wave-function \(\Psi = \sum_\alpha \psi_\alpha\), where \(\psi_\alpha\) are the components of the wave function given by the solution of the equation (3).

Splitting (4) of the potentials in general case is done in the three-body configuration space by the Merkuriev cut-off function \(\chi_\alpha [21]\)

\[
V^{(l)}_\alpha(x_\alpha, y_\alpha) = \chi_\alpha(x_\alpha, y_\alpha) V_\alpha(x_\alpha). \tag{5}
\]

This splitting confines the short-range part of the potential to the regions in the three-body configuration space corresponding to the three-body collision point (particles are close to each other) and the binary configuration \((x_\alpha \ll y_\beta, \text{ when } y_\beta \to \infty)\). The form of the cut-off function can be rather arbitrary within some general requirements [22]. Traditionally, the following form of the cut-off function proposed in [23] has been used

\[
\chi_\alpha(x_\alpha, y_\alpha) = 2/[1 + \exp[(x_\alpha/x_{0\alpha})^{16}/(1 + y_\beta/y_{0\beta})]]. \tag{6}
\]

The parameters \(x_{0\alpha}\) and \(y_{0\beta}\) can in principle be chosen arbitrarily, but their choice changes the properties of components \(\psi_\alpha\) that are important from both the theoretical and computational points of view [28]. The splitting procedure (4, 6) is done in the three-body configuration space and is suitable for energies either below the three-body breakup threshold or above this threshold. In the paper [24] we have shown, that for the energies below the disintegration threshold the splitting can be vastly simplified by confining the cut-off function \(\chi_\alpha(x_\alpha)\) to the two-body configuration space. Formally it is obtained by choosing \(y_{0\beta} = \infty\), which leads to

\[
\chi_\alpha(x_\alpha) = 2/[1 + \exp[(x_\alpha/x_{0\alpha})^{16}]]. \tag{7}
\]

With this smoothed Heaviside step function at \(\nu_\alpha = 2.01\) which is used in this paper for actual calculations, the split potentials \(V^{(s, l)}_\alpha\) become two-body quantities \(V^{(s, l)}_\alpha = V^{(s, l)}_\alpha(x_\alpha)\).
The splitting procedure makes the properties of the FM equations for Coulomb potentials as appropriate for scattering problems as standard Faddeev equations in the case of short-range potentials [11]. The key property of the FM equation (3) is that the right-hand side of each equation is confined to the vicinity of the triple collision point [28]. It results in the asymptotic uncoupling of the set of FM equations and, accordingly, the asymptote of each component \( \psi_i \) for energies below the breakup threshold contains only terms corresponding to binary configurations of pairing \( \alpha \) [11, 28]. For the total energy \( E \) of the system below the three-body ionization threshold it reads

\[
\psi_i (x_\alpha, y_\alpha) = \Phi^n \alpha (x_\alpha, y_\alpha) \delta_{\alpha,0} + \sum_A \frac{\phi_{\alpha A} (x_\alpha, y_\alpha)}{x_\alpha} Y_m (\hat{x}_\alpha) \left[ \frac{p_m}{P_0} \right] \times A_{A,\alpha} (y_\alpha) e^{i(p_0y_\alpha - y_\alpha \log(2\pi R_{\alpha,0}))} \frac{1}{y_\alpha},
\]

where the multi-index \( A = \{nlm\} \) specifies various two-body Coulomb bound states in the pair \( \alpha \) (that is, binary scattering channels \( \{\alpha; A\} \)) with the wave function \( \phi_{\alpha A} (x_\alpha, y_\alpha) / x_\alpha \) and the energy \( \varepsilon_\alpha \). Here \( Y_m (\hat{x}_\alpha) \) stands for the standard spherical harmonic function. The momentum \( p_m \) of the outgoing particle is determined by the energy conservation condition \( E = P_0^2 + \varepsilon_\alpha \) and the Sommerfeld parameter is defined as \( \eta_\alpha = Z_\alpha (Z_\alpha + 2 \sqrt{2m_p \varepsilon_\alpha} / 2p_0) \). The binary scattering amplitude \( A_{A,\alpha} (y_\alpha) \) corresponds to the transition from the initial binary channel \( \{\alpha; A\} \) to the binary channel \( \{\alpha; A\} \). The initial channel is specified by the incoming wave generated by the asymptotic Coulomb interaction between the projectile and the target \( V_{\text{eff}} (y_\alpha) = 2p_0 \eta_\alpha / y_\alpha (\beta, \gamma = \alpha) \)

\[
\Phi^n \alpha (x_\alpha, y_\alpha) = \frac{\phi_{\alpha nA} (x_\alpha, y_\alpha)}{x_\alpha} Y_{\eta_\alpha} (\hat{x}_\alpha) \times \delta^{(3)} (y_\alpha - S_{\alpha nA} p_m) e^\frac{i}{2} (1 + i) \frac{1}{y_\alpha} 
\]

where \( \delta^{(3)} \) is the confluent hypergeometric function [29].

The total angular momentum is an integral of motion for the three-particle system. This makes it possible to reduce the set of FM equations by projecting (3) onto a subspace of a given total angular momentum [9]. In this article we consider the case of zero total angular momentum of the system. The kinetic energy operator in the left-hand side of the equation (3) on the subspace of zero total orbital momentum has the form

\[
T_0 = \frac{\partial^2}{\partial x_\alpha^2} - \frac{2}{y_\alpha} \frac{\partial}{\partial y_\alpha} - \frac{2}{x_\alpha} \frac{\partial}{\partial x_\alpha} - \frac{1}{y_\alpha} \frac{\partial}{\partial z_{\alpha}} \left( 1 - z_{\alpha}^2 \right) \frac{\partial}{\partial z_{\alpha}},
\]

where \( z_{\alpha} \equiv \cos (\hat{x}_\alpha \cdot \hat{y}_\alpha) \). The corresponding projection of the component \( \psi_i \) depends only on the coordinates \( X_\alpha = \{x_\alpha, y_\alpha, z_{\alpha}\} \) in the plane containing all three particles. By choosing the coordinate system appropriately the projection of the asymptote (8) on the state with zero total angular momentum can be written as (the constant factor is omitted)

\[
\psi_i (X_\alpha) \sim - \frac{\phi_{\alpha nA} (x_\alpha)}{x_\alpha} Y_{\ell m} (\theta_\alpha, \phi_\alpha) e^{i\ell \phi_\alpha} e^{-i\ell \phi_\alpha} e^{i\ell \phi_\alpha} \delta_{\alpha,0} + \sum_{nA} \frac{\phi_{\alpha nA} (x_\alpha)}{x_\alpha} Y_{\ell m} (\theta_\alpha, \phi_\alpha) \left[ \frac{P_m}{P_0} \right] S_{nA,\alpha} e^{i\ell \phi_\alpha},
\]

where \( \psi_i (X_\alpha) \equiv \psi_i (x_\alpha, y_\alpha) \equiv \eta_\alpha \log (2p_0 y_\alpha) - \ell \pi / 2 + \sigma_\alpha \), \( \sigma_\alpha = \text{arg} \left( 1 + i \eta_\alpha \right) \) and \( S_{nA,\alpha} = \delta_{nA} e_{\alpha 0} + 2p_0 e^{-i\ell \phi_\alpha} e^{i\ell \phi_\alpha} e^{i\ell \phi_\alpha} A_{nA,\alpha} \) are the \( S \)-matrix elements. The total amplitude \( A_{A,\alpha} \) is related to partial amplitudes \( A_{nA,\alpha} \) according to

\[
\sum_{m=-\ell}^{\ell} \int d^2 \theta_\alpha |A_{A,\alpha} (\theta_\alpha)|^2 = 4\pi |A_{nA,\alpha}|^2 + \ldots,
\]

where the omitted terms at the right-hand side are the contributions from higher total angular momenta.

### 3. Numerical solution

To reduce the computational cost of solving the system of FM equations (3), several modifications have been made. At first, since the potential \( V_3 \) is repulsive and the corresponding two-body Hamiltonian does not support any bound states, this potential is included to the left-hand side of equation (3), thus reducing the number of equations from (3) to (2):

\[
\{T_0 + V_3 (x_\alpha) + V^{\text{eff}} (y_\alpha) + V_{\psi} (x_\alpha) - E\} \psi_i (x_\alpha) = -V^{\psi} (x_\alpha) \psi_i (x_\alpha),
\]

where \( \beta = x = 1, 2 \). Formally, it is done by setting \( \chi_3 = 0 \). Secondly, the asymptotic particle-atom Coulomb potential \( V_{\psi} (y_\alpha) \) is introduced explicitly in (13) for treating the asymptotic Coulomb singularity

\[
\{T_0 + V_3 (x_\alpha) + V^{\text{eff}} (y_\alpha) - E\} \psi_i (x_\alpha) = -V_{\psi} (x_\alpha) \psi_i (x_\alpha) - [V^{\psi} (x_\alpha) + V_3 (x_\alpha) - V^{\text{eff}} (y_\alpha)] \psi_i (x_\alpha).
\]

After that the Coulomb singularity can be effectively inverted as described below. Thirdly, it is more convenient to work with the modified components

\[
\tilde{\psi}_i (x_\alpha) = x_\alpha y_\alpha \psi_i (x_\alpha),
\]

that satisfy the system of equations

\[
\{\tilde{T}_0 + V_3 (x_\alpha) + V^{\text{eff}} (y_\alpha) - E\} \tilde{\psi}_i (x_\alpha) = -\frac{x_\alpha y_\alpha}{x_\alpha y_\alpha} \psi_i (x_\alpha) \times V_\alpha (x_\alpha) \tilde{\psi}_i (x_\alpha) - [V^{\psi} (x_\alpha) + V^{\text{eff}} (y_\alpha)] \tilde{\psi}_i (x_\alpha),
\]

\[
\tilde{T}_0 = \frac{\partial^2}{\partial x_\alpha^2} - \frac{\partial^2}{\partial x_\alpha^2} - \frac{1}{c^2} \frac{\partial}{\partial z_{\alpha}} \left( 1 - c^2 \right) \frac{\partial}{\partial z_{\alpha}},
\]

with \( \tilde{T}_0 = \frac{\partial^2}{\partial x_\alpha^2} - \frac{\partial^2}{\partial x_\alpha^2} \left( 1 + c^2 \right) \frac{\partial}{\partial z_{\alpha}} \left( 1 - c^2 \right) \frac{\partial}{\partial z_{\alpha}} \). The component \( \tilde{\psi}_i \) satisfies zero boundary conditions on the lines \( x_\alpha = 0, y_\alpha = 0 \) and the asymptotic boundary condition
obtained by multiplying formula (11) by $x_\alpha y_\alpha$, reads:

$$\psi_\alpha(x_\alpha) \sim -\phi_{\alpha n_\alpha l_\alpha}(x_\alpha)y_{0\alpha}(0, \theta_\alpha, 0) e^{-il\eta_\alpha(x_\alpha, p_{\alpha n_\alpha} s)} + \sum_{\alpha l_\alpha n_\alpha} \phi_{\alpha l_\alpha n_\alpha}(x_\alpha)y_{0\alpha}(0, \theta_\alpha, 0) \frac{P_{\alpha l_\alpha n_\alpha}}{P_{n_\alpha}} S_{\alpha l_\alpha n_\alpha} e^{-il\eta_\alpha(x_\alpha, p_{\alpha n_\alpha} s)}.$$  

(17)

Another modification is done to make the solutions of the equations (16) real functions. We recast (17) into the form

$$\psi_\alpha(x_\alpha) \sim -\phi_{\alpha n_\alpha l_\alpha}(x_\alpha)y_{0\alpha}(0, \theta_\alpha, 0) \sin(\phi_{\alpha l_\alpha}(x_\alpha, p_{\alpha n_\alpha} s)) \delta_{\alpha l_\alpha n_\alpha} + \sum_{\alpha l_\alpha n_\alpha} \phi_{\alpha l_\alpha n_\alpha}(x_\alpha)y_{0\alpha}(0, \theta_\alpha, 0) \frac{P_{\alpha l_\alpha n_\alpha}}{P_{n_\alpha}} K_{\alpha l_\alpha n_\alpha} \cos(\phi_{\alpha l_\alpha}(x_\alpha, p_{\alpha n_\alpha} s)).$$  

(18)

where the real numbers $K_{\alpha l_\alpha n_\alpha}$ form the $K$-matrix. One can show that a solution of the system of equations (16) with complex valued asymptotic boundary conditions (17) is a linear combination of its solutions with boundary conditions (18) (standing waves) with different initial channels $\{\alpha_0, A_0\}$. It gives the standard matrix relation between the $S$- and $K$-matrices

$$S = -(K + il)^{-1} \cdot (K - il).$$  

(19)

Here $I$ is the identity matrix of the rank equal to the number of open channels $N_{ch}$.

The boundary value problem (16), (18) is solved by the spline collocation method [25]. We solve equations in a box $[0, R_1^\alpha] \times [0, R_2^\alpha] \times [-1, 1]$ for each component $\psi_\alpha$. As a basis set for expanding the component we use the products of quintic Hermite splines $S_3^3$ (splines of degree 5 with 2 continuous derivatives) in each coordinate. Each basis function is local and nonzero only on two adjoining intervals of the grid. The boundary conditions (18) are implemented as follows. For each open channel $\{\alpha_0, A_0\}$ we construct the driven system of equations by making substitutions

$$\tilde{\psi}_\alpha(x_\alpha) = \psi_\alpha(x_\alpha) + \phi_{\alpha n_\alpha l_\alpha}(x_\alpha)S_{\alpha l_\alpha}(x_\alpha)y_{0\alpha}(0, \theta_\alpha, 0) \delta_{\alpha l_\alpha n_\alpha},$$  

(20)

where $S$ is the basis spline satisfying $S(R_{\alpha n_\alpha}^\alpha) = 1$:

$$(\tilde{T}_\alpha + V_{\alpha}(x_\alpha) + V_{\alpha}^{\text{eff}}(x_\alpha) - E) \tilde{\psi}_\alpha(x_\alpha) = -\frac{x_{\alpha l_\alpha} y_{\alpha j_\alpha}}{x_{\beta j_\beta}} \left \{ V_{\alpha}^{(0)}(x_\alpha) \tilde{\psi}_\beta(x_\beta) - [V_{\beta}^{(0)}(x_\beta) + V_{\beta}^{(1)}(x_\beta) - V_{\alpha}^{(1)}(x_\alpha)] \tilde{\psi}_\alpha(x_\alpha) + f_{\alpha}(x_\alpha), \alpha = 1, 2. \right.$$  

(21)

Here the inhomogeneous term is given by

$$f_{\alpha}(x_\alpha) = \phi_{\alpha n_\alpha l_\alpha}(x_\alpha)y_{0\alpha}(0, \theta_\alpha, 0) \left \{ -\frac{d^2}{dx_\alpha^2} + \ell_{\alpha}(\ell_{\alpha} + 1) \right \} \delta_{\alpha l_\alpha n_\alpha} + \frac{x_{\alpha l_\alpha} y_{\alpha j_\alpha}}{x_{\beta j_\beta}} V_{\alpha}^{(1)}(x_\alpha) \delta_{\alpha l_\alpha n_\alpha} S_{\alpha l_\alpha}(x_\alpha).$$  

(22)

The system of equations in (21) is supplied with zero boundary conditions $\tilde{\psi}_\alpha(x_\alpha) = 0$ on the sides of the box $[0, R_1^\alpha] \times [0, R_2^\alpha]$. The so obtained solution components $\tilde{\psi}_\alpha^{(\text{asym})}(x_\alpha)$, being a linear combination of physical solutions, behave asymptotically as

$$\tilde{\psi}_\alpha^{(\text{asym})}(x_\alpha) \sim \sum_{\alpha l_\alpha n_\alpha} \phi_{\alpha l_\alpha n_\alpha}(x_\alpha)y_{0\alpha}(0, \theta_\alpha, 0) \times (s_{\alpha l_\alpha n_\alpha} \sin(\phi_{\alpha l_\alpha}(x_\alpha, p_{\alpha n_\alpha} s)) + c_{\alpha l_\alpha n_\alpha} \cos(\phi_{\alpha l_\alpha}(x_\alpha, p_{\alpha n_\alpha} s))),$$  

(23)

with some coefficients $s_{\alpha l_\alpha n_\alpha}$ and $c_{\alpha l_\alpha n_\alpha}$. These coefficients can be extracted by projecting the function $\tilde{\psi}_\alpha^{(\text{asym})}$ at some distant point $x_\alpha$ on two-body bound states

$$\int_0^{R_2^\alpha} dx_\alpha \int_{-1}^1 d\cos \theta_\alpha \phi_{\alpha l_\alpha}(x_\alpha)y_{0\alpha}(0, \theta_\alpha, 0) \tilde{\psi}_\alpha^{(\text{asym})}(x_\alpha) = s_{\alpha l_\alpha n_\alpha} \sin(\phi_{\alpha l_\alpha}(x_\alpha, p_{\alpha n_\alpha} s)) + c_{\alpha l_\alpha n_\alpha} \cos(\phi_{\alpha l_\alpha}(x_\alpha, p_{\alpha n_\alpha} s)),$$

(24)

and using extrapolation. We obtain $N_{ch}$ solutions $\tilde{\psi}_\alpha^{(\text{asym})}$ of driven equations corresponding to different open channels $\{\alpha_0, A_0\}$ for a given total energy $E$. These solutions are linearly independent due to conditions $\tilde{\psi}_\alpha^{(\text{asym})}(x_\alpha) = \phi_{\alpha n_\alpha l_\alpha}(x_\alpha)y_{0\alpha}(0, \theta_\alpha, 0) \delta_{\alpha l_\alpha n_\alpha}$ at $X_\alpha = \{x_\alpha, R_1^\alpha, R_2^\alpha\}$. The solution of interest $\tilde{\psi}_\alpha^{(\text{asym})}$ is their linear combination. The formula linking $\tilde{\psi}_\alpha^{(\text{asym})}$ with the solutions $\tilde{\psi}_\alpha^{(\text{asym})}$ allows one to obtain all the $K$-matrix elements from the coefficients $s_{\alpha l_\alpha n_\alpha}$ and $c_{\alpha l_\alpha n_\alpha}$.

The equations in (21) are the final equations that are solved numerically. The components are expanded in terms of products of quintic Hermite splines:

$$\tilde{\psi}_\alpha(x_\alpha) = \sum_{\alpha j_\alpha k_\alpha} c_{\alpha j_\alpha k_\alpha} S_j(x_\alpha)S_k(y_\alpha)S_l(z_\alpha), \quad \alpha = 1, 2.$$  

(25)

Substituting the series (25) into equation (21) and requiring the resulting equalities to be satisfied in a number of points $(x_\alpha^j, y_\alpha^j, z_\alpha^j)$ of a rectangular grid one gets the matrix equation on coefficients $c_{\alpha j_\alpha k_\alpha}^\text{eff}$:

$$\begin{pmatrix} H_1 - ES \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ [H_2 - ES_2] \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \end{pmatrix},$$  

(26)

where the matrices $H_\alpha = \tilde{T}_\alpha + V_\alpha + V_\alpha^{\text{eff}}$ and

$$R = \begin{pmatrix} 0 & V_1^{(s)} \\ V_2^{(s)} & 0 \end{pmatrix},$$  

(27)

are discretized versions of the operators of the left- and the right-hand sides of the system (21). Here for example the matrix $V_\alpha$ has elements $V_\alpha(x_\alpha^j)S_j(x_\alpha^j)S_k(y_\alpha^j)S_l(z_\alpha^j)$ with rows enumerated by point numbers $\xi_\alpha^j$ and columns by basis function numbers $ijk$. Right preconditioning by its left-hand
side matrix turns the system of linear equation (26) into
\[
\begin{align*}
\{I - R \{ [S_1^{-1}H_1 - EI]^{-1}S_1^{-1} & \quad 0 \\
0 & \quad [S_2^{-1}H_2 - EI]^{-1}S_2^{-1} \}\} \\
\times (\vec{c}_1 \quad \vec{c}_2) = (f_1 \quad f_2)
\end{align*}
\]
(28)

This system of linear equations is solved by Arnoldi iterations in GMRES variant [30]. On each iteration of the algorithm the most computationally expensive operation is multiplication of the matrix of (28) by a vector. The matrix \(R\) is sparse, it has at most \(2 \times 6 \times 6 \times 6 = 432\) nonzero elements in a row due to the locality of the basis. To invert the matrix \([S_0^{-1}H_0 - EI]\) we use the algorithm which is known as ‘tensor trick’ or matrix decomposition method ([25, 26, 31]). It provides fast diagonalization of the matrix using its tensor product structure
\[
[S_0^{-1}H_0 - EI] = (S_0^{-1})^{-1}D_0^\phi \otimes I \otimes I \\
+ I \otimes (S_0^{-1})^{-1}D_0^\phi \otimes I + (S_0^{-1})^{-1}X_2S_0^\phi \otimes I \otimes I \\
+ I \otimes (S_0^{-1})^{-1}Y_2S_0^\phi \otimes I \cdot (I \otimes I \otimes (S_0^{-1})^{-1}D_0^\phi) \\
+ (S_0^{-1})^{-1}V_1S_0^\phi \otimes I \otimes I + I \otimes (S_0^{-1})^{-1}V_\alpha \otimes \xi \otimes \xi \\
\times S_0^\phi \otimes I - E I \otimes I \otimes I,
\]
(29)

where the matrices \(S_0^{\phi}, D_0^\phi, S_0^{\phi}, \ldots\) represent the ‘one-dimensional’ matrices of basis splines and their second derivatives at the collocation points in the respective coordinates. For example, \(D_0^{\phi}\) is a matrix with elements \(S_0^{\phi}(X_0^\phi)\) enumerated by indices \(i\) and \(\xi\). The matrices \(V_0, X_2, Y_2, \ldots\) are the diagonal matrices of pair and centrifugal potentials values. For a more detailed description of a method we refer the reader to [26].

At the end of this section we discuss the properties of the cut-off function (7). As it was stated in section 2, the choice of parameters of the cut-off function should provide the asymptotic decoupling of FM equations, which is a result of the so-called asymptotic filtering [24, 28]. The latter means that each ‘asymptotically decoupled’ equation at a given energy \(E < 0\)
\[
[T_\alpha + V_\alpha(x_\alpha) + \sum_{\beta = \alpha} V_\beta^{(0)}(x_\beta) - E \] \phi_\alpha = 0
\]
(30)
supports only those solutions which contain bound states of particles in the pair \(\alpha\) interacting by \(V_\alpha\) potential (if any) and does not support any bound states of the particles in other pairs \(\beta \neq \alpha\) interacting by potentials \(V_\beta^{(0)}\). Let \(V_\beta^{(0)}\) for \(\beta \neq \alpha\) be attractive. The potential \(V_\beta^{(0)}\) is plotted in figure 1. The ground state energy \(E_0^{(0)} < 0\) of the two particles interacting via this potential is marked with the horizontal line. The value of \(E_0^{(0)}\) is governed by the parameter \(x_{0,\beta}\). The bigger the parameter is, the weaker is the potential and the smaller is the absolute value of \(E_0^{(0)}\). If the energy \(E\) in (30) is less than \(E_0^{(0)}\) then the channels corresponding to the bound states supported by the potentials \(V_\beta^{(0)}\) are closed and the filtering condition is fulfilled. Thus, for a given total energy \(E\) and a given \(\beta\) the cut-off function parameter \(x_{0,\beta}\) should be bigger than some critical value \(x_0\) that is defined as follows: the ground state energy \(E_0^{(0)}\) of a two-body Hamiltonian with the potential \(V_\beta^{(0)}\) for \(x_{0,\beta} = x_0\) should be equal to \(E\). There is no upper bound on the values of \(x_{0,\beta}\), but we observed that the bigger is the value of the parameter, the bigger bases in angular coordinates are to be taken to obtain the desired accuracy. Summarizing, we

Figure 1. The long-range tail part of the potential \(V_\beta = -1/x_\beta\) obtained by using the cut-off function (7) with parameter \(x_{0,\beta} = 3.0\). The dotted line denotes the ground state energy level of two particles interacting by this potential.
propose the following algorithm of choosing the cut-off function parameter $x_{0,j}$:

(i) For a total energy interval $[E_{\min}, E_{\max}]$ of interest find the critical values of parameters $x_{0,j}$ for the total energy value $E_{\max}$ for each $\beta$.

(ii) Take the value of the parameter $x_{0,j}$ only slightly bigger than the critical value calculated at step (i).

4. Results

4.1. Scattering in $e^- e^+ \bar{p}$ and $e^+ e^- p$ systems

Positron–hydrogen atom scattering is the simplest example of positron–atom scattering process. Many calculations are presented in the literature, among them are detailed calculations using the FM equations for low energies [10, 12, 27] and the energies above the ionisation threshold [13]. Other methods include hyperspherical [7, 8], variational [2, 4] and close coupling calculations using two-center basis functions expansion [5, 6]. The renewed interest in studying the reactions involving positron, electron and (anti)proton is motivated by experiments on antimatter that take place at CERN [27]. The reaction of antihydrogen formation via antiproton ($\bar{p}$) impact of positronium ($Ps$, the bound state of $e^+ e^- p$) atom plays the key role in antimatter formation. Due to the symmetry in particle charges, the cross sections in $e^+ e^- p$ and $e^- e^+ \bar{p}$ systems are identical. Further in this section we refer to the $e^+ e^- \bar{p}$ system.

Solving the FM equations, we have calculated the $K$-matrix elements of all possible scattering processes in $e^+ e^- \bar{p}$ system in the total energy range between the $H(n = 1)$ and $H(n = 3)$ atom states energies, i.e. from $-0.49973$ to $-0.05553$ a.u. with the energy step of $0.0007$ a.u. Within this energy interval elastic scattering, excitation and rearrangement processes leading to $H(n = 1, 2)$ and $Ps(n = 1, 2)$ atom states are possible. The energy of these atom states form the thresholds for scattering channels. The maximum linear size of $K$-matrix equals to 6, corresponding to 6 open channels in the interval between energies of $Ps(n = 2)$ and $H(n = 3)$ states. We proceed as follows: the whole energy region is divided into subintervals associated with the energy thresholds in the system. For every interval we choose appropriate discretisation and cut-off function parameters according to the rules described in the previous section. This is done to minimize computational costs, since calculations at higher energies require

- bigger box sizes in $x_o$, $y_o$ and more basis functions involved;
- bigger cut-off parameters $x_{0,\alpha}$, that in turn put stronger requirements for the angular coordinate basis.

The energy intervals and the corresponding discretisation and cut-off function parameters are given in table 1. In this table and further in the text we use shortcuts $H(n)$ and $H(n, \ell)$ for the atom states with the principal quantum number $n$ and the angular momentum $\ell$. The parameters are found by the coordinate descent algorithm which was used to minimize the cross section computational errors and make them less than 1%.

In table 2 we show the convergence of different cross sections at the energy $E = -0.0572$ a.u., which belongs to the energy interval corresponding to the last column of table 1, and asymmetry of the $K$-matrix. The latter is defined as

$$R = \frac{|\langle K - K^T \rangle|}{||K||}$$

with the Frobenius norm of a matrix. We demonstrate the convergence with respect to a given parameter while the values of other parameters are fixed to those given in the last column of table 1.

Besides the obvious fact that the bigger is the value of each parameter the better is the accuracy we see in table 2 in the different convergence rate of cross sections and asymmetry, the cross sections are already stable within three significant digits, whereas the value of asymmetry is of $10^{-1}$ order. The further improvement of asymmetry by an order of magnitude and more is reached by increasing of $x_0$ parameter of the cut-off function. However, this does not change noticeably the values of cross sections leaving the cross sections accuracy practically within the same range. This situation is typical for all energy regions of table 1 and it was used for the final choice of parameters in table 1 as a compromise between the required accuracy and the computational complexity.

In table 3 we compare our results with tabulated results of other authors and give the values of some additional cross sections for further references. The agreement between our results and that of other calculations is quite good. The only noticeable disagreement is in some values of cross sections for $H(1)$ formation, our results being a few percent lower than that of other authors. We note that the calculation of $H(1)$ formation amplitudes should be done with extra accuracy, otherwise it may be prone to errors. The reason is that the

| First component | $H(1)$–$Ps(1)$ | $Ps(1)$–$H(2)$ | $H(2)$–$H(3)$ |
|-----------------|----------------|----------------|----------------|
| $x_{\max}$     | 17.7           | 28.3           | 70.7           |
| $y_{\max}$     | 42.4           | 84.9           | 141            |
| $n_x$           | 45             | 60             | 75             |
| $n_y$           | 120            | 300            | 510            |
| $n_z$           | 24             | 24             | 24             |
| $x_0$           | 1.4            | 3.5            | 8.5            |

| Second component | $H(1)$–$Ps(1)$ | $Ps(1)$–$H(2)$ | $H(2)$–$H(3)$ |
|-----------------|----------------|----------------|----------------|
| $x_{\max}$     | 35             | 70             | 100            |
| $y_{\max}$     | 17.5           | 35             | 115            |
| $n_x$           | 60             | 75             | 75             |
| $n_y$           | 60             | 105            | 600            |
| $n_z$           | 18             | 30             | 45             |
| $x_0$           | 1              | 4              | 8              |
## Table 2. Convergence of cross sections for scattering in e\(e^+\) system with respect to components \(\psi_1\) (left) and \(\psi_2\) (right) discretization and cut-off function parameters, total energy \(E = -0.057\ 2286\ a.u\).

We use the notation \(Ps, H, e\) to specify the reaction \(\psi_1 \rightarrow \psi_2\) and similar notations for other reactions.

### Energy and Components

| \(E\) (a.u.) | \(\psi_1\) | \(\psi_2\) |
|-------------|-------------|-------------|
| 0.057       | 11.65       | 11.75       |
| 0.113       | 11.65       | 11.75       |
| 0.170       | 11.65       | 11.75       |

### Cross Sections

| \(\sigma\) (a.u.) | \(R(1 \rightarrow \psi_1)\) | \(R(1 \rightarrow \psi_2)\) |
|------------------|---------------------------|---------------------------|
| 0.55             | 11.65                     | 11.75                     |
| 1.00             | 11.65                     | 11.75                     |
| 1.50             | 11.65                     | 11.75                     |

### Additional Parameters

- \(\pi_1\) and \(\pi_2\) are the components of the polarization vectors.
- \(\alpha_1\) and \(\alpha_2\) are the polar angles with respect to the incident electron.
- \(\beta_1\) and \(\beta_2\) are the azimuthal angles.

### References

- Gradusov, V.A. et al. J. Phys. B: At. Mol. Opt. Phys. 62 (2019) 055202.
Table 3. Scattering cross sections in $e^{-}e^{+}\bar{p}$ system, present results and that of other authors (the energy is measured from the $-0.499$ 73 a.u. $\bar{H}(1)$ threshold.

| $E$, a.u. | 0.270 26 | 0.281 40 | 0.320 17 | 0.361 45 | 0.385 | 0.40 | 0.415 | 0.42 |
|-----------|-----------|-----------|-----------|-----------|-------|------|-------|------|
| $\sigma_{e^{-}+\bar{H}(1)\rightarrow e^{+}+\bar{H}(1)}$ | 0.0353 | 0.0417 | 0.0634 | 0.0836 | 0.0944 | 0.100 | 0.105 | 0.107 |
| [5] | | | | | 0.0651 | 0.0844 | 0.100 | |
| [10] | | | | | 0.0431 | 0.0650 | 0.0856 | |
| $\sigma_{e^{-}+\bar{H}(1)\rightarrow \bar{\beta}+Ps(1)}$ | 0.00412 | 0.00430 | 0.00487 | 0.00562 | 0.00565 | 0.00572 | 0.00575 | 0.00574 |
| [5] | | | | | 0.00490 | 0.00567 | 0.00581 | |
| [10] | | | | | 0.00410 | 0.00439 | 0.00487 | 0.00557 |
| [4] | | | | | 0.00422 | 0.00481 | 0.00554 | |
| $\sigma_{Ps(1)\rightarrow \bar{\beta}+Ps(1)}$ | 3.49 | 7.06 | 9.87 | 8.31 | 7.11 | 6.44 | 5.82 | 5.62 |
| [5] | | | | | 9.87 | 8.32 | 6.45 | |
| [10] | | | | | 3.500 | 7.060 | 9.866 | 8.312 |
| [4] | | | | | 6.936 | 9.868 | 8.332 | |
| $\sigma_{\bar{\beta}+Ps(1)\rightarrow e^{-}+\bar{H}(1)}$ | 0.0272 | 0.0191 | 0.0111 | 0.0091 | 0.00806 | 0.00763 | 0.00724 | 0.00709 |
| [10] | | | | | 0.0274 | 0.0195 | 0.0111 | 0.0091 |
| $\sigma_{\bar{H}(1)\rightarrow e^{-}+\bar{H}(2,\ell)}$ | | | | | | | | |
| $\sigma_{\bar{H}(1)\rightarrow e^{-}+\bar{H}(2,p)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(1)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(2)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(3)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(1)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(2)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(3)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(4)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(5)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(6)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(7)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(8)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(9)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(10)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(11)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(12)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(13)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(14)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(15)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(16)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(17)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(18)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(19)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(20)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(21)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(22)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(23)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(24)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(25)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(26)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(27)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(28)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(29)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(30)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(31)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(32)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(33)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(34)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(35)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(36)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(37)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(38)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(39)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(40)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(41)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(42)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(43)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(44)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(45)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(46)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(47)}$ | | | | | | | | |
| $\sigma_{\bar{H}(2,\ell)\rightarrow \bar{\beta}+Ps(48)}$ | | | | | | | | |
The cross sections for processes leading to He\(^{+}\) and \(\bar{H}\)\(^{+}\) states are large, for example the cross sections in the energy region near threshold were also found recently in [36, 37]. According to [36, 37] the energy position \(E_n\) of the \(n\)th maximum of the oscillations must follow the rule

\[
\log(E_n - E_{th}) = An + B,
\]

where \(A\) and \(B\) are constants and \(E_{th}\) is the threshold energy. We plot the respective quantities for \(\bar{p} + Ps(1) \rightarrow e^- + \bar{H}(1)\) and \(\bar{p} + Ps(1) \rightarrow e^- + \bar{H}(2)\) near threshold oscillations in figure 4. Clearly, the linear spacing of \(\log(E_n - E_{th})\) is near perfect in both cases of rearrangement cross sections except for the last points. The latter can indicate the range of validity of approximations made in [36, 37] leading to (31). As for the behavior of the \(\bar{p} + Ps(2) \rightarrow e^- + \bar{H}(n \leq 2)\) cross section on the right panel of figure 3, we obviously cannot make such quantitative analysis of above the Ps(2) threshold oscillations. Nevertheless, we can agree with [27] that there is an oscillation with the energy position close to \(-0.061\) 94 a.u., which was also found earlier in [38]. It should be noted that the elastic cross section oscillations for Ps–p scattering above Ps(2) threshold were also found recently in [39].

4.2. scattering in \(e^+e^-\)He\(^{++}\) system

Positron-positive helium ion is an example of positron–atomic target scattering in which asymptotic Coulomb interaction is present in one of the configurations. There are a number of calculations in a wide energy region, among them are close coupling calculations using two center basis functions expansion [40, 41] and EFS-CDW method [42]. But to the best of our knowledge, there is lack of published results of calculation for the low-energy region. In this work solving the FM equations we have calculated \(K\)-matrices of all possible scattering processes in \(e^+e^-\)He\(^{++}\) system in the total energy range between the energy thresholds of He\(^{+}\) (1) and He\(^{+}\) (4) states, i.e. from \(-1.9997\) to \(-0.124\) 96 a.u. with the energy step of calculation 0.0007 a.u. In this interval elastic, excitations and rearrangement processes leading to He\(^{+}\) (\(n = 1, 2, 3\)) and Ps(\(n = 1\)) atom states are possible. The maximum linear size of the \(K\)-matrix equals 7. We proceeded as in the case of \(e^+e^-\) \(\bar{p}\) system, using different sets of discretisation and cut-off function parameters for subsequent energy intervals between the thresholds. These intervals

\[\text{Figure 3. Antihydrogen formation cross sections. Black triangles mark points given in [27].} \]
and corresponding parameters are given in table 4. We have found that the convergence of our calculations for $e^+e^-He^{++}$ system is quite similar to that of $-\bar{e}eHe^{++}$ system and therefore we do not give here an analog of table 2. As in the previous case we hold the accuracy of calculations of cross sections within the error range not exceeding 1%.

The calculated values of 11 of all 49 cross sections are given in table 5. The dependence on energy of cross sections for the reactions $e^-He^+\rightarrow e^-He^+$, $e^-He^+\rightarrow He^{++}-Ps$ and $He^{++}-Ps\rightarrow He^{++}-Ps$, $He^{++}-Ps\rightarrow e^-He^+$ is displayed in figure 5. The largest cross sections are, as in the case of $e^-e^-He^{++}$ system, the elastic ground state positronium cross section and those that are associated with excited helium ion states.

All scattering cross sections associated with non excited atom states follow the well known laws of threshold behavior [43], which are presented briefly in table 6 where $p$ means the relative momentum between the target and the projectile. The only exception is the cross section for $e^+ + He^+ (1) \rightarrow He^{++} + Ps(1)$ process (dark-magenta line in figure 5). At the $-0.25$ a.u. threshold, according to table 6,

![Figure 4](image_url)

**Figure 4.** (a), (b)—detailed plots of $\bar{p} + Ps(1) \rightarrow e^- + \bar{H}(1)$ and $\bar{p} + Ps(1) \rightarrow e^- + \bar{H}(2)$ cross sections in the energy region above the $\bar{H}(2)$ threshold. For these cross sections, the logarithm of the relative energy positions $log(E_n - E_0)$ of oscillations maxima with respect to their numbers $n$ are depicted in figures (c)–(e).

| First component | He$^+(1)$-He$^+(2)$ | He$^+(2)$-Ps(1) | Ps(1)-He$^+(4)$ |
|-----------------|----------------------|-----------------|-----------------|
| $x_{max}$       | 10.6                 | 21.2            | 35.4            |
| $y_{max}$       | 35.4                 | 99              | 120             |
| $n_x$           | 60                   | 60              | 90              |
| $n_y$           | 270                  | 810             | 960             |
| $n_z$           | 15                   | 27              | 21              |
| $x_0$           | 2.1                  | 2.8             | 5.8             |

| Second component |
|------------------|
| $x_{max}$        | 15                  | 50              | 60              |
| $y_{max}$        | 7.5                 | 20              | 35              |
| $n_x$            | 60                   | 90              | 105             |
| $n_y$            | 60                   | 120             | 195             |
| $n_z$            | 15                   | 18              | 42              |
| $x_0$            | 1                    | 1               | 3.5             |
it should tend to zero linearly as \( p \to 0 \), but it grows up to some constant value instead. This anomaly can be regarded as a sign of a near threshold resonance, see the discussion below. The near \( \text{He}^+ (2) \) threshold oscillations of cross sections for \( \text{He}^+ \) excitation to \( \text{He}^+(2, s) \) and \( \text{He}^+(2, p) \) reactions (green and blue lines in figure 5) are evidently due to their very small values being disturbed by numerical errors. The threshold behavior of scattering cross sections associated with excited atom states is more complicated due to the degeneracy of energy levels and requires special treatment \([36, 44, 45]\).

**Table 5.** Scattering cross sections in \( e^- e^+ \text{He}^+ \) system (the energy is measured from the \(-1.9997\) a.u. \( \text{He}^+(1) \) threshold). We use \( a(b) \) for \( a \times 10^b \).

| \( E \), a.u. | 1.55 | 1.60 | 1.65 | 1.70 | 1.77 | 1.80 | 1.83 | 1.86 |
|----------------|------|------|------|------|------|------|------|------|
| \( \sigma_{e^- + \text{He}^+(1) \to e^- + \text{He}^+(1)} \) | 0.000 855 | 0.001 01 | 0.001 16 | 0.001 33 | 0.001 58 | 0.001 68 | 0.001 78 | 0.001 88 |
| \( \sigma_{e^- + \text{He}^+(1) \to e^- + \text{He}^+(2,s)} \) \sim 1\((-9)\) | \sim 1\((-8)\) | 2\((-7)\) | 6\((-7)\) | 2.6\((-6)\) | 4.4\((-6)\) | 6.9\((-6)\) | 1.1\((-5)\) |
| \( \sigma_{e^- + \text{He}^+(1) \to e^- + \text{He}^+(2,p)} \) \sim 1\((-10)\) | \sim 1\((-8)\) | 3\((-7)\) | 2.5\((-6)\) | 1.1\((-5)\) | 1.8\((-5)\) | 2.6\((-5)\) | 3.6\((-5)\) |
| \( \sigma_{e^- + \text{He}^+(1) \to \text{He}^+ + \text{P}(1)} \) | 1\((-7)\) | 1\((-7)\) | 2\((-7)\) | 3\((-7)\) | |
| \( \sigma_{\text{He}^+ + \text{P}(1) \to \text{He}^+ + \text{P}(1)} \) | 20.6 | 19.6 | 8.82 | 3.00 | |
| \( \sigma_{\text{He}^+ + \text{P}(1) \to \text{e}^- + \text{He}^+(2,s)} \) | 0.366 | 0.102 | 0.0433 | 0.0199 | |
| \( \sigma_{\text{He}^+ + \text{P}(1) \to \text{e}^- + \text{He}^+(2,p)} \) | 0.094 4 | 0.0214 | 0.008 76 | 0.005 84 | |
| \( \sigma_{e^- + \text{He}^+(2,s) \to \text{e}^- + \text{He}^+(2,s)} \) | 1.12 | 3.35 | 6.64 | 6.63 | 5.11 | 4.59 | 4.10 | 3.66 |
| \( \sigma_{e^- + \text{He}^+(2,p) \to \text{e}^- + \text{He}^+(2,p)} \) | 5.34 | 4.57 | 2.76 | 1.35 | 0.866 | 0.832 | 0.820 | 0.815 |
| \( \sigma_{\text{He}^+ + \text{X}_1 \to \text{He}^+(2,s)} \) | 9.87 | 18.4 | 11.7 | |
| \( \sigma_{\text{He}^+ + \text{X}_1 \to \text{He}^+(2,p)} \) | 15.7 | 1.62 | 1.21 | |

**Figure 5.** Cross sections in \( e^- e^+ \text{He}^+ \) system. Vertical solid lines denote binary thresholds, vertical dashed lines mark resonance positions. We use the notation \( Ps(n_1, ℓ_1) \to \text{He}^+(n_2, ℓ_2) \) to specify the reaction \( \text{He}^{++} + Ps(n_1, ℓ_1) \to e^- + \text{He}^+(n_2, ℓ_2) \) and similar notations for other reactions. (This figure is in colour only in the electronic version.)

**Table 6.** Threshold behavior of cross sections in the system of two compound particles \( a \) and \( X \), for elastic scattering and rearrangement to \( b \) and \( Y \). \( p \) is the relative momentum of incoming or outgoing slow particles, either oppositely charged or not charged, the angular momentum of the system equals to zero \([43]\).

| Process | Not charged | Charged |
|---------|-------------|---------|
| Elastic | Const | \( 1/p^2 \) |
| slow \to fast rearrangement | \( 1/p \) | \( 1/p^2 \) |
| fast \to slow rearrangement | \( p \) | const |
Table 7. Broad resonance in the e+e−He++ system energies (E∗, Γ) (in a.u.).

| Present work  | (−0.3704, 0.1297) | (−0.1857, 0.0395) |
|---------------|------------------|------------------|
| Gailitis [47]  | (−0.3705, 0.1294) | (−0.1856, 0.0393) |

For e+e−He++ system, resonance energies are worse known, there exist a number of disagreements between results [46–48] (and references therein). Most authors agree that there are two broad resonances at −0.371 and −0.188 a.u. [47] and one narrow resonance slightly below the positronium ground state formation threshold at −0.250 a.u. [47, 48]. Positions of these resonances are marked in figure 5 by dashed vertical lines (dashed vertical line at −0.250 a.u. almost coincides with vertical line denoting the positronium ground state threshold and is not visible). We do not see the usual singular behavior in the cross sections in the vicinity of the narrow resonance. However, the anomalous threshold behavior of the e+ + He− (1) → He++ + Ps(1) cross section at Ps(1) threshold, as discussed above, can indicate the presence of a resonance. Broad resonances are not seen in the cross sections expected.

To check the existence of broad resonances we have used another approach based on the complex rotation method applied to the Schrödinger equation [49]. We have found these broad resonances, their positions and widths are given in table 7 and compared with results of [47].

The sharp local minimum is again seen in the He++ + Ps(1) → He− + + Ps(1) cross section (royal blue line in figure 5) for the direct process with neutral target. Again, we associate this minimum with the Ramsauer–Townsend effect.

5. Conclusions
In this paper the detailed calculations of low-energy reactive scattering in e−e−p and e−e−He++ systems for the zero total angular momentum have been performed with the use of the FM equations in total angular momentum representation. The total angular momentum representation for FM equations assumes all partial waves in subsystems to be included in the formalism, thus, in this respect the obtained results should be considered complete.

The calculated cross sections in e−e−p system reproduce all the known resonant peaks. The sharp minima in elastic cross sections p − Ps(n = 1) and He− − Ps(n = 1) at low relative energies display the Ramsauer–Townsend effect. The Gailitis–Damburg oscillations of the p + Ps(1) → e− + H(1) and p + Ps(1) → e− + H(2) cross sections just above the H(2) threshold are discovered and the proper spacing of the oscillation maxima with respect to the threshold is verified.

The two known broad resonances [47] in e−e−He++ system do not contribute into the cross section profile. We suggest to explain the anomalous threshold behavior of the e+ + He− (1) → He++ + Ps(1) cross section by the existence of the narrow resonance found in [47, 48].

We have demonstrated that FM equations formalism is efficient for calculating elastic and reactive scattering in three body atomic systems. We hope that it will also be useful tool for studying three-body configurations in different physical applications.

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