Faddeev–Merkuriev integral equations for atomic three-body resonances

S Keller, A Marotta and Z Papp

Department of Physics and Astronomy, California State University Long Beach, Long Beach, CA, USA

Received 4 August 2008, in final form 16 October 2008
Published 3 February 2009
Online at stacks.iop.org/JPhysB/42/044003

Abstract

Three-body resonances in atomic systems are calculated as complex-energy solutions of Faddeev-type integral equations. The homogeneous Faddeev–Merkuriev integral equations are solved by approximating the potential terms in a Coulomb–Sturmian basis. The Coulomb–Sturmian matrix elements of the three-body Coulomb Green’s operator have been calculated as a contour integral of two-body Coulomb Green’s matrices. This approximation casts the integral equation into a matrix equation and the complex energies are located as the complex zeros of the Fredholm determinant. We calculated resonances of the $e–Ps$ system at higher energies and for total angular momentum $L = 1$ with natural and unnatural parity.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The wavefunction of a three-particle system is very complicated. It may have several different kinds of asymptotic behaviour reflecting the possible asymptotic fragmentations. It is very hard to impose all the asymptotic conditions on a single wavefunction. The Faddeev approach is a simplification: the wavefunction is split into components such that each component describes only one kind of asymptotic fragmentation [1]. Then only one kind of asymptotic behaviour should be imposed on each component. The components satisfy a set of coupled equations, the Faddeev equations.

If we want to apply this idea to systems with Coulomb potentials, we may run into difficulties. The Coulomb potential is a long-range potential, thus the motion in a Coulomb field never becomes a free motion, even at asymptotic distances. Consequently, the separation of the wavefunction along different asymptotic properties does not really work. If we just plug the Coulomb potential into the original Faddeev equations, the equations become singular. The usual asymptotic analysis fails to provide the boundary condition. In integral equation form, the kernel of the equations fails to be compact and we cannot approximate them by finite-rank terms.

Merkuriev proposed [1, 2] a modification of the Faddeev procedure which led to integral equations with compact kernels and differential equations with known boundary conditions.

Resonances are related to the outgoing-wave solutions of the Schrödinger equation at complex energies $E = E_r - i\Gamma/2$. Here $E_r$ is the resonance energy and $\Gamma$ is the resonance width, which is related to the lifetime of the decaying state. In an integral equation formalism, the resonances are the solutions of the homogeneous integral equations on the unphysical sheet, close to real energies.

A few years ago, a method for solving Faddeev-type integral equations for scattering problems [3] was adopted to calculate resonances [4]. The homogeneous version of the Faddeev integral equations was solved at complex energies on the unphysical sheet. The method entails expanding the potentials terms in the integral equations on a Coulomb–Sturmian basis. This transforms the integral equations to a matrix equation. $S$-wave resonances of the $e–Ps$ system have been calculated and good agreement with the results of methods based on complex rotation of the coordinates was found [5, 6].

An accumulation of resonance poles around thresholds has been reported in [7]; however, we do not investigate these threshold resonances here. They are either too close to the threshold, too close to each other, or too broad as we move away from the threshold. In any case, their experimental verification does not seem to be likely in the near future.

In this paper, we will report some new developments of this method. In section 2, we will outline the Faddeev–Merkuriev approach to the three-body Coulomb problem. In section 3, we detail the Coulomb–Sturmian separable expansion approach. We introduce a new contour integral for the three-body Green’s operator which makes the analytic continuation to the resonance region easier. In section 4, we
present resonances of the e–P system three-body system up to the fifth threshold with total angular momentum \( L = 1 \). We provide results for both natural and unnatural parity states.

2. Faddeev–Merkuriev integral equations

The Hamiltonian of an atomic three-body system is given by

\[
H = H^0 + v_1^C + v_2^C + v_3^C ,
\]

where \( H^0 \) is the three-body kinetic energy operator and \( v_\alpha^C \) denotes the Coulomb interaction of each subsystem \( \alpha = 1, 2, 3 \). Throughout, we use the usual configuration-space Jacobi coordinates \( x_\alpha \) and \( y_\alpha \), where \( x_\alpha \) is the distance between the pair \( (\beta, \gamma) \) and \( y_\alpha \) is the distance between the centre of mass of the pair \( (\beta, \gamma) \) and the particle \( \alpha \). Thus, the potential \( v_\alpha^C \), the interaction of the pair \( (\beta, \gamma) \), appears as \( v_\alpha^C(x_\alpha) \). In an atomic three-body system, two particles always have the same sign of charge. So, without loss of generality, we can assume that they are particles 1 and 2, and therefore \( v_3^C \) is a repulsive Coulomb potential.

The Hamiltonian (1) is defined in the three-body Hilbert space. Therefore, the two-body potential operators are formally embedded in the three-body Hilbert space,

\[
v_\alpha^C = v_\alpha^C(x_\alpha)1_{y_\alpha},
\]

where \( 1_{y_\alpha} \) is a unit operator in the two-body Hilbert space associated with the \( y_\alpha \) coordinate.

The role of a Coulomb potential in a three-body system is twofold. The Coulomb potential is a long-range potential but it also possesses some features of a short-range potential. It strongly correlates the particles and may even support two-body bound states. These two properties are contradictory and require different treatment. Merkuriev proposed a separation of the three-body configuration space into different asymptotic regions [2]. The two-body asymptotic region \( \Omega_\alpha \) is defined as a part of the three-body configuration space where the conditions

\[
(|x_\alpha|/\lambda_0)^\nu < |y_\alpha|/\lambda_0
\]

with parameters \( \lambda_0 > 0, \lambda_0 > 0 \) and \( \nu > 1 \) are satisfied. It was shown that in \( \Omega_\alpha \), the short-range character of the Coulomb potential prevails, while in the complementary region the long-range character of the Coulomb potential becomes dominant. Thus, it seems to be a good idea to split the Coulomb potential in the three-body configuration space into short-range and long-range terms

\[
v_\alpha^C = v_\alpha^{(s)}(x_\alpha) + v_\alpha^{(l)}(x_\alpha),
\]

where the superscripts \( s \) and \( l \) indicate the short- and long-range attributes, respectively. The splitting is carried out with the help of a splitting function \( \zeta_\alpha \).

\[
v_\alpha^{(s)}(x_\alpha, y_\alpha) = v_\alpha^C(x_\alpha)\zeta_\alpha(x_\alpha, y_\alpha),
\]

\[
v_\alpha^{(l)}(x_\alpha, y_\alpha) = v_\alpha^C(x_\alpha)[1 - \zeta_\alpha(x_\alpha, y_\alpha)].
\]

The function \( \zeta_\alpha \) vanishes asymptotically within the three-body sector, where \( x_\alpha \sim y_\alpha \to \infty \), and approaches 1 in the two-body asymptotic region \( \Omega_\alpha \), where \( x_\alpha \ll y_\alpha \to \infty \).

As a result, in the three-body sector, \( v_\alpha^{(s)} \) vanishes and \( v_\alpha^{(l)} \) approaches \( v_\alpha^C \). In practice, the functional form

\[
\zeta_\alpha(x_\alpha, y_\alpha) = 2/[1 + \exp[(x_\alpha/x_0)^\nu/(1 + y_\alpha/y_0)]]
\]

is used. Typical shapes for \( v^{(s)} \) and \( v^{(l)} \) are shown in figures 1 and 2, respectively.

In the Hamiltonian (1) the Coulomb potential \( v_3^C \) is repulsive and does not support bound states. Consequently, there are no two-body channels associated with this fragmentation and the entire \( v_3^C \) can be considered as long-range potential. Then the long-range Hamiltonian is defined as

\[
H^l(l) = H^0 + v_1^{(l)} + v_2^{(l)} + v_3^C ,
\]

and the three-body Hamiltonian takes the form

\[
H = H^0 + v_1^{(l)} + v_2^{(l)}.
\]

This Hamiltonian looks like an ordinary three-body Hamiltonian with two short-range interactions.

To determine the bound and resonant states, we have to solve the Schrödinger equation

\[
H|\Psi\rangle = E|\Psi\rangle
\]

for real and complex \( E \) eigenvalues, respectively. In the Faddeev approach the Faddeev components are defined by

\[
|\psi_\alpha\rangle = (E - H^0)^{-1}v_\alpha^{(l)}|\Psi\rangle,
\]

where \( \alpha = 1, 2 \). This involves a splitting of the wavefunction into two components

\[
|\Psi\rangle = |\psi_1\rangle + |\psi_2\rangle .
\]
Then for the Faddeev components, we have the set of equations, the Faddeev equations,
\[
\begin{align*}
(E - H^{(1)}) \psi_1 &= v^{(1)}_1 \psi_2, \\
(E - H^{(2)}) \psi_2 &= v^{(2)}_2 \psi_1.
\end{align*}
\]
where
\[
H^{(1)}_0 = H^{(1)} + v^{(1)}_0.
\]
By adding these two equations and taking into account equation (12) we recover the original Schrödinger equation. So, the Faddeev procedure is no more and no less than a method of solving the Schrödinger equation. We can cast these differential equations into an integral equation form
\[
\begin{align*}
|\psi_1| &= G^{(1)}_1(E) v^{(1)}_1 |\psi_2|, \\
|\psi_2| &= G^{(2)}_2(E) v^{(2)}_2 |\psi_1|,
\end{align*}
\]
where
\[
G^{(1)}_1(E) = (E - H^{(1)}_0)^{-1}.
\]
Before going further, we should examine the spectral properties of the Hamiltonian
\[
H^{(1)}_0 = H^{(1)} + v^{(1)}_0 = H^0 + v^C + v^{(1)}_1 + v^{(1)}_2.
\]
It is obvious that it supports infinitely many two-body channels associated with the bound states of the attractive Coulomb potential \(v^C\). Potential \(v^C\) is repulsive, therefore does not support bound states and there are no two-body channels associated with fragmentation 3. The three-body potential \(v^{(2)}_1\) is attractive. It is a valley along a parabola-like curve which becomes shallower and shallower, and finally disappears as \(y_2\) goes to infinity (see figure 2). Thus, \(v^{(2)}_1(\tau, y_2)\) does not support two-body bound states either in the subsystem \(\tau, y_2\) if \(y_2 \to \infty\). Consequently, there are no two-body channels associated with fragmentation 2. Therefore, the asymptotic Hamiltonian \(H^{(1)}_0\) has two-body channels only in the fragmentation where particle 1 is at infinity and particles 2 and 3 form bound states. If either particle 2 or 3 is at infinity, no bound states are allowed in the respective subsystem. The corresponding \(G^{(1)}_1\) Green’s operator, acting on the \(v^{(1)}_1 |\psi_2|\) term in (16), will generate only those two-body channels in \(|\psi_1|\) where particle 1 is at infinity and particles 2 and 3 form bound states. A similar analysis is also valid for \(|\psi_2|\).

So, the Merkuriev procedure results in a separation of the three-body wavefunction into components in such a way that each component has only one type of two-body channel. This is the main advantage of the original Faddeev equations and, as the above analysis shows, this property remains valid also for attractive Coulomb potentials.

The long-range part of the Coulomb potential, \(v^{(l)}_0\), does not support two-body channels. It may, however, support bound states, i.e. \(H^{(1)}_0\) may have three-body bound states. This can lead to the appearance of spurious solutions of the Faddeev–Merkuriev equations. If \(H^{(1)}_0\) has a bound state, then \((z - H^{(1)}_0)^{-1}\) is singular at this energy. Consequently, in equation (11), applying this singular operator on a vanishing \(|\Psi|\) may produce a non-vanishing \(|\psi_1\rangle\). So, we may find a solution where neither \(|\psi_1\rangle\) nor \(|\psi_2\rangle\) vanishes, but \(|\Psi|\) = \(|\psi_1\rangle + |\psi_2\rangle\) vanishes. These states would be non-trivial solutions of the Faddeev–Merkuriev equations, but would be trivial solutions of the original Schrödinger equation. These states are spurious, or ghost, solutions. A way to eliminate them is to ensure that in the energy range of physical interest \(H^{(1)}_0\) does not have bound states. We can achieve this by choosing the parameters \(x_0\) and \(y_0\) accordingly. For resonances at higher energies we should take a bigger \(x_0\), thus pushing the unwanted bound states of \(H^{(1)}_0\) out of the spectrum of physical interest. It is also obvious from this analysis that the spurious solutions are sensitive to the choice of \(x_0\) and \(y_0\), while the true resonances are not. By varying the parameters \(x_0\) and \(y_0\), one can single out the possible spurious solutions.

A very nice advantage of the Faddeev equations is that the identity of particles simplifies the equations. If particles 1 and 2 are identical particles, the Faddeev components \(\psi_1\) and \(\psi_2\), in their own natural Jacobi coordinates, must have the same functional forms
\[
\langle x_1 y_1 |\psi_1 | = \langle x_2 y_2 |\psi_2 |.
\]
On the other hand, by interchanging particles 1 and 2, we have
\[
\mathcal{P}_{12} |\psi_1 | = \sigma |\psi_2 |,
\]
which by itself determines \(|\psi_1 |\). We note that so far no approximation has been made, and even though this integral equation has only one component, it gives a full account of the asymptotic and symmmetry properties of the system.

3.3. Separable expansion solution of the Faddeev equations

3.1. Coulomb–Sturmian basis

The Coulomb–Sturmian (CS) functions [8] are the solutions of the Sturm–Liouville problem of the Coulomb Hamiltonian
\[
\left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2b(n+1+l)}{r} + b^2\right) r^l |n; b\rangle = 0,
\]
where \(b\) is a parameter, \(n\) is the radial quantum number and \(l\) is the angular momentum. In configuration space, the CS functions are given by
\[
\langle r| n; b\rangle = \frac{n!}{(n+2l+1)!} \exp(-br)(2br)^l L_n^{(2l+1)}(2br),
\]
where \(L_n\) denotes the Laguerre polynomials. By defining the functions \(|r| n; b\rangle = (\langle r| n; b\rangle)/r\), the orthogonality and completeness relations take the forms
\[
|n\rangle| n; b\rangle = |n\rangle| n; b\rangle = \delta_{nn'},
\]
and
\[
1 = \lim_{N \to \infty} \sum_{n=0}^N \langle n; b\rangle| n; b\rangle = \lim_{N \to \infty} \sum_{n=0}^N \langle n; b\rangle| n; b\rangle. (25)
\]
Since the three-body Hilbert space is a direct product of two-body Hilbert spaces, an appropriate basis is the bipolar
basis, which can be defined as the angular-momentum-coupled direct product of the two-body bases,
\[ |n\nu l; b_x b_y\rangle_a = |n l; b_x\rangle_a \otimes |\nu \lambda; b_y\rangle_a,\]

where \(|n l; b_x\rangle_a\) and \(|\nu \lambda; b_y\rangle_a\) are associated with the coordinates \(x_a\) and \(y_a\), respectively. With this basis, the completeness relation takes the form (with angular momentum summation implicitly included)
\[ 1 = \lim_{N \to \infty} \sum_{n,\nu l; b_x b_y} |n\nu l; b_x b_y\rangle_a \langle n\nu l; b_x b_y|_a = \lim_{N \to \infty} 1^N_a, \]

where \(|xy n\nu l; b_x b_y\rangle = (xy) |n\nu l; b_x b_y\rangle_a/(xy)\).

3.2. Separable approximation

We may introduce a unit operator into the Faddeev equation
\[ |\psi_1\rangle = \lim_{N \to \infty} G_1^{(l)}(E) 1^N_a v^N_0 \langle 1^N_a | \psi_2\rangle \]
\[ |\psi_2\rangle = \lim_{N \to \infty} G_2^{(l)}(E) 1^N_a v^N_0 \langle 1^N_a | \psi_1\rangle. \]

This identity becomes an approximation if we keep \(N\) finite, which is the equivalent of approximating \(v^N_0\) in the three-body Hilbert space by a separable form
\[ v^{(s)}_0 = \lim_{N \to \infty} 1^N_a v^{(s)}_0 \approx 1^N_a v^{(s)}_0 1^N_a \approx \sum_{n,\nu l; b_x b_y} |n\nu l; b_x b_y\rangle_a \tilde{v}^{(s)}_{a
u l; b_x b_y} \langle n\nu l; b_x b_y.\]

where \(\tilde{v}^{(s)}_{a
u l; b_x b_y} = \langle n\nu l; b_x b_y \rangle_a v^{(s)}_0 \langle n'\nu' l'; b_x b_y\rangle_b\). These matrix elements can be evaluated numerically by using the transformation of the Jacobi coordinates [9]. The completeness of the CS basis guarantees the convergence of the expansion with increasing \(N\) and angular momentum channels.

Now, by applying the bra \(|n'\nu' l'\rangle_b\) from the left, the solution of the homogeneous Faddeev–Merkuriev equation turns into the solution of a matrix equation for the component vector
\[ \tilde{\psi}_1 = G^{(l)}_1(E) \tilde{v}^{(s)}_0 \tilde{\psi}_2, \]
\[ \psi_1 = G^{(l)}_2(E) \tilde{v}^{(s)}_0 \psi_2, \]

where
\[ G^{(l)}_a = a |n\nu l; b_x b_y\rangle |G^{(l)}_a| n'\nu' l'; b_x b_y\rangle_a. \]

These equations can be transformed into the matrix form
\[ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} G^{(l)}_1(E) & 0 \\ 0 & G^{(l)}_2(E) \end{bmatrix} = 0, \]

which exhibits a homogeneous algebraic equation for the Faddeev components. This homogeneous algebraic equation is solvable if and only if
\[ D(E) = \text{det} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} G^{(l)}_1(E) & 0 \\ 0 & G^{(l)}_2(E) \end{bmatrix} = 0, \]

where \(D(E)\) is the Fredholm determinant. The real-energy solutions provide us with the bound states, while the complex-energy ones give the resonant states.

3.3. Calculation of \(G^{(l)}_a\)

Unfortunately, the Green’s operator \(G^{(l)}_a\) is not known. It is related to the asymptotic Hamiltonian \(H^{(l)}_a\), which is still a complicated three-body Coulomb Hamiltonian. However, \(H^{(l)}_a\) has only one type of two-body asymptotic channels where particle \(a\) is at infinity. This asymptotic Hamiltonian is denoted by \(H^{(l)}_{a\infty}\). If a three-body system has only one type of asymptotic channel, then a single Lippmann–Schwinger equation provides a unique solution:
\[ G^{(l)}_a(z) = G^{as}_a(z) + G^{as}_a(z) V^{as}_a G^{(l)}_a(z), \]

where \(G^{as}_a(z)\) is an asymptotic channel Green’s operator, \(G^{as}_a(z) = (z - H^{as}_a)^{-1}\), and \(V^{as}_a = H^{as}_a - H^{as}_{a\infty}\). Merkuriev constructed \(G^{as}_a\) in the different asymptotic regions of the three-body configuration space and showed that the kernel of this Lippmann–Schwinger equation is completely continuous (compact) [1, 2]. Therefore, \(V^{as}_a\) can also be approximated by a separable form
\[ V^{as}_a = \lim_{N \to \infty} 1^N_a V^{as}_a 1^N_a \approx 1^N_a v^{as}_a 1^N_a \approx \sum_{n,\nu l; b_x b_y} |n\nu l; b_x b_y\rangle_a V^{as}_a \langle n'\nu' l'; b_x b_y,\]

where \(\tilde{v}^{as}_a = a |n\nu l; b_x b_y\rangle |V^{as}_a| n'\nu' l'; b_x b_y\rangle_a\). The solution of equations (36) can be expressed formally as
\[ (G^{(l)}_a)^{-1} = (G^{as}_a)^{-1} - V^{as}_a, \]

where
\[ G^{as}_a = a |n\nu l; b_x b_y\rangle |G^{as}_a| n'\nu' l'; b_x b_y\rangle_a, \]
\[ V^{as}_a = a |n\nu l; b_x b_y\rangle |V^{as}_a| n'\nu' l'; b_x b_y\rangle_a. \]

The matrix elements (39) and (40) have to be calculated between a finite number of square-integrable CS states. In these integrals, the CS functions, as a function of \(x_a\), decay exponentially for large \(x_a\). Hence the domain of integration is confined to \(\Omega_a\), where \(x_a\) is either finite, or \(x_a \ll y_a\) as \(y_a \to \infty\). In this region, as Merkuriev showed [2], \(G^{as}_a\) takes a simple form; it coincides with the channel Coulomb Green’s operator
\[ G^{as}_a = \tilde{G}_a, \]

where \(\tilde{G}_a(z) = (z - \tilde{H}_a)^{-1}\) and \(\tilde{H}_a = H^{as}_a + v^{as}_C\). Therefore, in calculating the matrix elements in equation (39), \(G^{as}_a\) can be replaced by \(\tilde{G}_a\). Similarly, in calculating (40), \(V^{as}_a\) can be replaced by
\[ U_a = v^{(l)}_a + v^{as}_C. \]

Consequently, equation (38) becomes
\[ (G^{(l)}_a)^{-1} = (\tilde{G}_a)^{-1} - U_a. \]
where
\[
\tilde{G}_\alpha = \{n^\nu \lambda; b_\lambda \} \tilde{G}_\alpha \{n'^\nu' \lambda'; b_\lambda \}_\alpha
\]
and
\[
U_\alpha = \{n^\nu \lambda; b_\lambda \} U_\alpha \{n'^\nu' \lambda'; b_\lambda \}_\alpha.
\]
The \(U_\alpha\) matrix elements can again be evaluated numerically.

3.4. Matrix elements of \(\tilde{G}_\alpha\)

The most crucial point in this procedure is the calculation of the matrix elements \(\tilde{G}_\alpha\). In our Jacobi coordinates, the three-particle free Hamiltonian can be written as a sum of two-particle free Hamiltonians
\[
H^0 = h^0_x + h^0_y.
\]
Thus, the Hamiltonian \(\tilde{H}_\alpha\) of equation (42) appears as a sum of two two-body Hamiltonians acting on different coordinates
\[
\tilde{H}_\alpha = h_x + h_y,
\]
where \(h_x = h^0_x + v_x(x)\) and \(h_y = h^0_y\), which, of course, commute. As a result, \(\tilde{G}_\alpha\) is a resolvent of the sum of two commuting Hamiltonians \(h_x\) and \(h_y\).

According to the Dunford–Taylor functional calculus, a function of a self-adjoint operator \(h\) can be defined by
\[
f(h) = \frac{1}{2\pi i} \oint_C dz' f(z' - h)^{-1},
\]
where \(C\) encircles the spectrum of \(h\) in counterclockwise direction and \(f\) is analytic on the area encircled by \(C\). In that way, \(\tilde{G}_\alpha\), as a function of the self-adjoint operator \(h_x\), can be written as
\[
\tilde{G}_\alpha(z) = (z - h_x)^{-1}
\]
where \(g_{\nu\lambda}(z) = (z - h_x)^{-1}\) and \(g_{\nu\lambda}(z) = (z - h_x)^{-1}\). The contour \(C\) should be taken in a counterclockwise direction around the singularities of \(g_{\nu\lambda}\) such that \(g_{\nu\lambda}\) is analytic on the domain encircled by \(C\). Accordingly, to calculate the matrix elements \(\tilde{G}_\alpha\), we need to calculate a contour integral of the two-body Green’s matrices \(g_{\nu\lambda}\) and \(g_{\lambda\nu}\).

In our case, \(g_{\nu\lambda}\) is a Coulomb Green’s operator with a branch-cut on the \([0, \infty)\) interval and accumulation of infinitely many bound states at zero energy, while \(g_{\lambda\nu}\) is a free Green’s operator with a branch-cut on the \([0, \infty)\) interval. In time-independent scattering theory, \(\tilde{G}_\alpha(E)\) should be understood as \(\tilde{G}_\alpha(E) = \lim_{\epsilon \to 0} \tilde{G}_\alpha(E + i\epsilon)\) with \(\epsilon > 0\). To calculate resonances, we need to continue analytically to \(\epsilon < 0\). In this paper, we limit our study to energies below the three-body breakup threshold, so \(\Re(E) < 0\).

To examine the analytic structure of the integrand in equation (50) let us take \(\epsilon > 0\). By doing so, the singularities of \(g_{\nu\lambda}\) and \(g_{\lambda\nu}\) become well separated. Now the spectrum of \(g_{\nu\lambda}\) can easily be encircled so that the singularities of \(g_{\nu\lambda}\) lie outside the encircled domain (figure 3). However, this would not be the case for \(\epsilon \leq 0\). Therefore the contour \(C\) is deformed analytically in such a way that it shrinks to a few lowest bound states and the contour opens up and continues along an imaginary line (figure 4). Now, even in the \(\epsilon < 0\) case (figure 5), the contour avoids the singularities of \(g_{\nu\lambda}\). Thus, the mathematical conditions for the contour integral representation of \(\tilde{G}_\alpha\) in equation (50) are met also for resonant-state energies.

3.5. The Coulomb–Sturmian matrix elements of the Coulomb Green’s operator

In our system, \(g_{\nu\lambda}\) is a free Green’s operator and \(g_{\nu\lambda}\) is a Coulomb Green’s operator. Their CS matrix elements can be
calculated analytically \[10\]. The two-body Coulomb Green’s operator is the resolvent of the Coulomb Hamiltonian 
\[ \tilde{g}_f^C = (z - h_i^C)^{-1}, \] (51)
where 
\[ h_i^C = -\frac{\hbar^2}{2m} \left( \frac{d^2}{dr^2} - \frac{l(l + 1)}{r^2} \right) + \frac{Z}{r}, \] (52)
m is the reduced mass and Z is the strength of the Coulomb potential. In the CS basis the operator \( J = z - h_i^C \) has an infinite symmetric tri-diagonal (Jacobi) matrix structure, i.e. all elements are zero, except for the diagonals and off-diagonals,
\[ J_{ii}^C = 2(i + l + 1)(k^2 - b^2) \frac{\hbar^2}{4mb} - Z, \] (53)
\[ J_{i-1}^C = -(i + 2l + 1)^{1/2}(k^2 + b^2) \frac{\hbar^2}{4mb}, \] (54)
and
\[ J_{ii+1}^C = -[(i + 1)(i + 2l + 2)]^{1/2}(k^2 + b^2) \frac{\hbar^2}{4mb}, \] (55)
where \( k = (2mZ/\hbar^2)^{1/2} \). Then, as has been shown in \[10\], the \( N \times N \) matrix elements of \( g_0^C \) are given by
\[ \tilde{J}_0^{C(N)} = \left[ J_C - \delta_{ij} \delta_{N,N'} \left( J_{N+1}^C \right)^2 \right] C_{N+1}, \] (56)
where \( J_C \) is the \( N \times N \) upper left corner of the Jacobi matrix and 
\[ C_{N+1} = -\frac{4m/\hbar^2 b}{(b - ik)^2 (N + l + 2 + iy)} \times 2F_1 \left(-l + iy, N + 2; N + l + 3 + iy; \left( \frac{b + ik}{b - ik} \right)^2 \right) \times 2F_1 \left(-l + iy, N + 1; N + l + 2 + iy; \left( \frac{b + ik}{b - ik} \right)^2 \right), \] (57)
with \( 2F_1 \) being the hypergeometric function and \( \gamma = Z/(m\hbar^2 k) \). This ratio of two \( 2F_1 \) functions, where the second and third indices in the numerator and in the denominator differ by 1, can be represented by a continued fraction \[11\], which is easily computable and convergent on the whole complex \( k \) plane.

3.6. Numerical realization of the method

In this approach for solving the Faddeev–Merkuriev integral equation, the only approximation is the replacement of the potentials \( v_i^{(l)} \) and \( U_{ix} \) by their separate separable forms. We found that good results are achieved when we use \( N \) up to 25–30 in the separable expansion for each angular momentum channel. To calculate the matrix elements between CS functions, which are, in fact, exponential functions multiplied by polynomials, we use Gaussian integration; about 120–150 points provide the sufficient accuracy.

The calculation of \( \tilde{G}_f \) is very accurate. It should be noted first that this representation of \( g_C^0 \) is exact, and its numerical realization, including the evaluation of the ratio of two \( 2F_1 \) functions by a continued fraction is precise to machine accuracy. The contour integral around the poles of \( g_{\alpha} \) is a projection onto the corresponding bound state
\[ | \phi_i \rangle \langle \phi_i | = \frac{1}{2\pi i} \oint_{C_i} dz \: g_{\alpha}(z), \] (58)
where \( \phi_i \) is the eigenstate belonging to the eigenvalue \( E_i \) and \( C_i \) is a contour around \( E_i \). In fact, the states \( | \phi_i \rangle \) are hydrogenic bound states. We calculated the overlap \( \langle nll;b(\phi_i) \rangle \) using (58) and compared it with the exact result in Maple. We found a perfect agreement. We also found that the main contribution to \( \tilde{G}_f \) is due to the bound-state poles. The contour integral along the imaginary line behaves asymptotically like \( 1/(1+z)^2 \). We adopted the Gauss-rational integration method, and found that about 50–60 integration points provide a sufficient accuracy. This is a significant improvement over previous methods which employed as many as 250 integration points in \[4, 7\] to achieve a comparable level of accuracy.

In order to find those complex zeros of \( D(E) \), which are close to the real energy line, we have developed the following procedure. We consider an interval along the real energy line between two thresholds. Since \( D(E) \) is an analytic function of the energy we can approximate it with Chebyshev polynomials. We use about \( n = 12–15 \) Chebyshev polynomials. The length of the interval should be small enough that \( D(E) \) does not change too much and thus the Chebyshev approximation is reliable. The zeros of the Chebyshev-approximated function are determined by using the eigenvalue method of \[12\]. Then the rank of the Chebyshev approximation is lowered by one, and the zeros are located again. If a zero is a true zero of \( D(E) \), the zeros of the rank \( n \) and rank \( n - 1 \) Chebyshev polynomials are close. A similar concept was adopted in \[13\] using Padé approximation instead of Chebyshev. We then look for the zeros of \( D(E) \) in the neighbourhood of the zeros of the Chebyshev approximation. We pick three complex points, \( z_1, z_2 \) and \( z_3 \). The location \( z_0 \) of the complex root is estimated by \[14\]
\[ z_0 = \zeta_1(z_2-z_3)/D(z_2)+\zeta_2(z_1-z_3)/D(z_1)+\zeta_3(z_1-z_2)/D(z_3), \] (59)
where \( \zeta_1, \zeta_2 \) and \( \zeta_3 \) are hydrogenic basis states. We then make a replacement \( z_0 \rightarrow z_1, z_1 \rightarrow z_2 \) and \( z_2 \rightarrow z_3 \), and repeat until \( |z_0 - z_1| < \epsilon \) with some small \( \epsilon \). If the initial estimation for the zero is good, this procedure converges very fast. After some experience, we found this method quite fast and reliable.

4. Results

We calculated the resonances of the electron–positronium, e–Ps or e−e–e+3, three-body system. Here the two electrons are identical particles, allowing us to use the one-component version of the homogeneous Faddeev–Merkuriev equations \[21\]. We use atomic units throughout. For the parameters of the cut-off function \( \gamma \) we adopted \( x_0 = 30, y_0 = 35 \) and \( v = 2.1 \). This choice of parameters guarantees that in the energy region up to the fifth threshold, there are no spurious solutions.

The parity of the states is given by \( P = (-)^l \). If \( P = (-)^l \), the state has natural parity, if \( P = (-)^{l+1} \), the state has unnatural parity. The wavefunction should be antisymmetric with respect to the exchange of the two electrons. If the spin of the two electrons couples to \( S = 0 \) to form a singlet state, then the wavefunction is antisymmetric with respect to the exchange of electron–spin coordinates, and the spatial part should be symmetric. Similarly, if the two electrons couple to
Table 1. Angular momentum channels $l - \lambda$ used for $L = 1$ states with natural and unnatural parity. The superscript stands for the parity.

| $L = 1^-$ | $L = 1^+$ |
|-----------|-----------|
| 0–1       | 1–0       |
| 1–0       | 2–2       |
| 1–2       | 3–3       |
| 2–1       | 4–4       |
| 2–3       | 5–5       |
| 3–2       | 6–6       |
| 3–4       | 7–7       |
| 4–3       | 8–8       |

Table 2. The convergence of a resonant-state energy with increasing $N$. The results are given in atomic units. $E_r$ is the real part and $E_i$ is the imaginary part of the energy.

| $N$ | $E_r$ | $E_i$ |
|-----|-------|-------|
| 25  | −0.028 958 565 292 | −0.000 000 304 662 |
| 26  | −0.028 959 758 422 | −0.000 000 303 622 |
| 27  | −0.028 960 583 605 | −0.000 000 302 855 |
| 28  | −0.028 961 155 544 | −0.000 000 302 318 |
| 29  | −0.028 961 553 239 | −0.000 000 301 934 |
| 30  | −0.028 961 831 103 | −0.000 000 301 642 |

For $S = 1$ forming a triplet state, the wavefunction is symmetric with respect to exchange of the spin coordinates, and the spatial part of the wavefunction is antisymmetric. Consequently, in equation (21), if $S = 0$ then $p = 1$ and if $S = 1$ then $p = −1$.

We present results for total angular momentum $L = 1$. The angular momentum quantum numbers $l$ and $\lambda$ are selected such that $\vec{l} + \vec{\lambda} = \vec{L}$. Table 1 shows the angular momentum channels used in these calculations.

In this method, we represent operators on the CS basis, which has one parameter, the parameter $b$. To be economic, we need to find an optimal $b$, and then we need to increase the basis size $N$ to observe convergence. We found that the results are insensitive to varying $b$ over a rather broad interval around $b = 0.25$. We used $b = 0.25$ throughout. Table 2 shows a typical convergence of a resonant-state energy with increasing $N$. From results like this, we can safely infer about three significant digits for the real part of energy and one or two significant digits for the imaginary part of the energy. Tables 3 and 4 show the results of our calculations.

5. Summary

In this paper, we outlined a solution method for the homogeneous Faddeev–Merkuriev integral equations to calculate resonances in atomic three-body systems. We approximated the potential terms in the three-body Hilbert space by a separable form. This approximation casts the integral equations into a matrix equation and the resonances are sought as complex-energy roots of the Fredholm determinant. The matrix elements of the three-body channel Coulomb Green’s operator were evaluated as a complex contour integral of the two-body Coulomb Green’s matrices. The use of the Coulomb–Sturmian basis allows analytic evaluation of these matrix elements. We found that the contour introduced here is more advantageous than those used in our previous publications [4, 7]. The method is quite efficient. To achieve good accuracy we do not need too many terms in the expansion, only $N = 30$ in each angular momentum channel, and consequently the size of the matrix is relatively small. We performed all of our calculations with Mac PCs. We calculated resonances of the $e$–$Ps$ atomic three-body system for total angular momentum $L = 1$ with natural and unnatural parity. We do not believe that there is an ultimate method for calculating resonances. However, our results allow us to believe that this solution of the homogeneous Faddeev–Merkuriev equations is an accurate and reliable method for calculating resonances in atomic three-body systems.

Acknowledgments

The authors are grateful to S L Yakovlev for useful discussions. This work has been supported by the Research Corporation.

References

[1] Faddeev L D and Merkuriev S P 1993 Quantum Scattering Theory for Several Particle Systems (Dordrecht: Kluwer)
[2] Merkuriev S 1980 Ann. Phys., NY 130 395
[3] Papp Z 1997 Phys. Rev. C 55 1080
  Papp Z, Hu C-Y, Hlousek Z T, Konya B and Yakovlev S L 2001 Phys. Rev. A 63 062721
[4] Papp Z, Darai J, Hu C-Y, Hlousek Z T, Konya B and Yakovlev S L 2002 Phys. Rev. A 65 032725
  Papp Z, Darai J, Nishimura A, Hlousek Z T, Hu C-Y and Yakovlev S L 2002 Phys. Lett. A 304 36
[5] Ho Y K 1984 Phys. Lett. 102A 348
[6] Li T and Shakeshaft R 2005 Phys. Rev. A 71 052505
[7] Papp Z, Darai J, Mezei J Zs, Hlousek Z T and Hu C-Y 2005
  Phys. Rev. Lett. 94 143201
  Mezei J Zs and Papp Z 2006 Phys. Rev. A 73 030701
[8] Rotenberg M 1962 Ann. Phys., NY 19 262
  Rotenberg M 1970 Adv. At. Mol. Phys. 6 233
[9] Balian R and Brézin E 1969 Nuovo Cimento B 2 403
[10] Demir F, Hlousek Z T and Papp Z 2006 Phys. Rev. A 74 014701
[11] Lorentzen L and Waadeland H 1992 Continued Fractions with Applications, Studies in Computational Mathematics vol 3
  (Amsterdam: North-Holland) pp 293–301
[12] Boyd J P 2006 J. Eng. Math. 56 203
[13] Rakityansky S A, Soñanos S A and Elander N 2007 J. Phys. A: Math. Theor. 40 14857
[14] Giraud B G, Mihailovic M V, Lovas R G and Nagarajan M A 1982 Ann. Phys., NY 140 29