Accumulation of three-body resonances above two-body thresholds

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We calculate resonances in three-body systems with attractive Coulomb potentials by solving the homogeneous Faddeev-Merkuriev integral equations for complex energies. The equations are solved by using the Coulomb-Sturmian separable expansion approach. This approach provides an exact treatment of the threshold behavior of the three-body Coulombic systems. We considered the negative positronium ion and, besides locating all the previously known S-wave resonances, we found a whole bunch of new resonances accumulated just slightly above the two-body thresholds. The way they accumulate indicates that probably there are infinitely many resonances just above the two-body thresholds, and this might be a general property of three-body systems with attractive Coulomb potentials.

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The most common method for calculating resonant states in quantum mechanical systems is the one based on the complex rotation of coordinates. The complex rotation turns the resonant behavior of the wave function into a bound-state-like asymptotic behavior. Then, standard bound-state methods become applicable also for calculating resonances. The complex rotation of the coordinates does not change the discrete spectrum, the branch cut, which corresponds to scattering states, however, is rotated down onto the complex energy plane, and as a consequence, resonant states from the unphysical sheet become accessible. By changing the rotation angle the points corresponding to the continuum move, while those corresponding to discrete states, like bound and resonant states, stay. This way one can determine resonance parameters. In three-body systems there are several branch cuts associated with two-body thresholds.

In practice, the complex rotational technique is combined with some variational approach. This results in a discretization of the rotated continuum. The points of the discretized continuum scatter around the rotated-down straight line. So, especially around thresholds it is not easy to decide whether a point is a resonance point or it belongs to the rotated continuum. Moreover, variational methods approach states from above, so resonances slightly above the thresholds may easily get lost.

Recently, we have developed a method for calculating resonances in three-body Coulombic systems by solving homogeneous Faddeev-Merkuriev integral equations using the Coulomb-Sturmian separable expansion approach. As a test case, we calculated the resonances of the negative positronium ion. This system has been extensively studied in the past two decades and thus serves as test example for new methods. We found all the 12 S-wave resonances presented in Ref. and observed good agreements in all cases.

We also observed that in case of attractive Coulomb interactions the Faddeev-Merkuriev integral equations may produce spurious resonances, which are related to the somewhat arbitrary splitting of the potential in the three-body configuration space into short-range and long-range terms. We could single them out by changing those parameters. We succeeded in locating 10 more resonances in the same energy region, all of them are very close to the thresholds. These new resonances were published in Ref.

As our skill in applying our method developed we located more and more new resonances just slightly above the two-body thresholds. They are all aligned along a line in the complex energy plane pointing toward the thresholds. It seems that there are infinitely many resonances accumulating at the two-body thresholds. Since our method is relatively new we briefly outline the basic concepts and the numerical techniques, specialized to the e⁻e⁻e⁺ system (further details are in Refs.

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

\[ H = H^0 + v^C_1 + v^C_2 + v^C_3, \]

where \( H^0 \) is the three-body kinetic energy operator and \( v^C_\alpha \) denotes the Coulomb potential in the subsystem \( \alpha \), with \( \alpha = 1, 2, 3 \). We use throughout the usual configuration-space Jacobi coordinates \( x_\alpha, y_\alpha \), where \( x_\alpha \) is the coordinate of the \((\beta, \gamma)\) pair and \( y_\alpha \) connects the center of mass of \((\beta, \gamma)\) to the particle \( \alpha \), respectively. Thus \( v^C_\alpha \), the potential between particles \( \beta \) and \( \gamma \), depends on \( x_\alpha \).

The Hamiltonian \( H \) is defined in the three-body Hilbert space. The three-body kinetic energy, when the center-of-mass motion is separated, is given by

\[ H^0 = h^0_{x_\alpha} + h^0_{y_\alpha} = h^0_{x_\alpha} + h^0_{y_\beta} = h^0_{x_\alpha} + h^0_{y_\gamma}, \]

where \( h^0 \) is the two-body kinetic energy. The two-body potential operators are formally embedded in the three-body Hilbert space \( v^C = v^C(x)1_y \), where \( 1_y \) is a unit operator in the two-body Hilbert space associated with the \( y \) coordinate.

In Merkuriev’s approach to the three-body Coulomb problem the Coulomb interaction is split, in the three-body configuration space, into short- and long-range terms

\[ v^C_\alpha = v^{(s)}_\alpha + v^{(l)}_\alpha, \]

where \( v^{(s)}_\alpha \) and \( v^{(l)}_\alpha \) represent the short-range and long-range parts of the potential, respectively.
The components are defined by Faddeev-Merkuriev integral equations
\[ v_\alpha^{(s)} = v_\alpha^C \zeta(x_\alpha, y_\alpha) \]
\[ v_\alpha^{(l)} = v_\alpha^C [1 - \zeta(x_\alpha, y_\alpha)] . \]
The splitting function \( \zeta \) is defined such that
\[ \lim_{x,y \to \infty} \zeta(x,y) = \begin{cases} 1, & \text{if } |x| < x_0 (1 + |y|/y_0)^{1/\nu}, \\ 0, & \text{otherwise}, \end{cases} \]
where \( x_0, y_0 > 0 \) and \( \nu > 2 \). So, in the region of three-body configuration space where particles \( \beta \) and \( \gamma \) are close to each other \( v_\alpha^{(s)} \sim v_\alpha^C \) and \( v_\alpha^{(l)} \sim 0 \), otherwise \( v_\alpha^{(l)} \sim v_\alpha^C \) and \( v_\alpha^{(s)} \sim 0 \). Usually the functional form
\[ \zeta(x,y) = 2 \left\{ 1 + \exp \left[ (x/x_0)^\nu / (1 + y/y_0) \right] \right\}, \]
is used. Typical picture for \( v^{(s)} \) and \( v^{(l)} \) are seen in Fig. 1.

In atomic three-particle systems the sign of the charge is always identical for two particles. Let us denote those two particles by 1 and 2, and the third one by 3. In this case \( v^{(s)} \) is a repulsive Coulomb potential which does not support two-body bound states. Therefore the entire \( v^{(s)} \) can be considered as long-range potential and the Hamiltonian can formally be written in a form which looks like an usual three-body Hamiltonian with two short-range potentials
\[ H = H^{(l)} + v^{(s)} + v^{(s)} + v^{(s)}, \]
where the long-range Hamiltonian is defined as
\[ H^{(l)} = H^{(l)} + v^{(l)} + v^{(l)} + v^{(l)} \]

Then, the Faddeev method is applicable and, in this particular case, results in a splitting of the wave function into two components
\[ |\Psi\rangle = |\psi_1\rangle + |\psi_2\rangle. \]
The components are defined by \( |\psi_\alpha\rangle = G^{(l)}(z)|v^{(s)}\rangle |\Psi\rangle \), where \( \alpha = 1, 2 \) and \( G^{(l)}(z) = (z - H^{(l)})^{-1}, z \) is a complex number.

In the cases of bound and resonant states the wave-function components satisfy the homogeneous two-component Faddeev-Merkuriev integral equations
\[ |\psi_1\rangle = G^{(l)}(z)v^{(s)}|\psi_2\rangle \]
\[ |\psi_2\rangle = G^{(l)}(z)v^{(s)}|\psi_1\rangle , \]
at real and complex energies, respectively. Here \( G^{(l)}(z) \) is the resolvent of the channel long ranged Hamiltonian \( G^{(l)}(z) = (z - H^{(l)})^{-1}, \)

Further simplification can be achieved if we take into account that particles 1 and 2 are identical and indistinguishable. Then, the Faddeev components \( |\psi_1\rangle \) and \( |\psi_2\rangle \), in their own natural Jacobi coordinates, have the same functional forms \( \langle x_1 y_1 | \psi_1 \rangle = \langle x_2 y_2 | \psi_2 \rangle \). On the other hand \( |\psi_2\rangle = p P |\psi_1\rangle \), where \( P \) is the operator for the permutation of indexes 1 and 2 and \( p = \pm 1 \) denotes the eigenvalue of \( P \). Therefore we can determine \( |\psi_1\rangle \) from the first equation only
\[ |\psi_1\rangle = G^{(l)}(z) v^{(s)} p P |\psi_1\rangle. \]

It should be noted, that so far we did not make any approximation, and although this integral equation has only one component, yet it gives full account both of asymptotic and symmetry properties of the system.

We solve Eq. (13) by using the Coulomb–Sturmian separable expansion approach. The Coulomb-Sturmian (CS) functions are defined by
\[ \langle r | n l \rangle = \frac{n!}{(n + 2l + 1)!} (2br)^{l+1} \exp(-br)L_n^{2l+1}(2br), \]
\( n \) and \( l \) are the radial and orbital angular momentum quantum numbers, respectively, and \( b \) is the size parameter of the basis. The CS functions \( \{ | n l \rangle \} \) form a biorthonormal discrete basis in the radial two-body Hilbert space; the biorthogonal partner is defined by \( \langle r | n l \rangle = \langle r | n l \rangle / r \). Since the three-body Hilbert space is a direct product of two-body Hilbert spaces an appropriate basis can be defined as the angular momentum coupled direct product of the two-body bases
\[ | n \nu l \lambda \rangle = | n \lambda \rangle \otimes | n \lambda \rangle, \quad (n, \nu = 0, 1, 2, \ldots) \]
where \( | n \lambda \rangle \) and \( | n \lambda \rangle \) are associated with the coordinates \( x_1 \) and \( y_1 \), respectively. With this basis the completeness relation takes the form
\[ 1 = \lim_{N \to \infty} \sum_{n, \nu = 0}^{N} \langle n \nu l \lambda | n \nu l \lambda \rangle = \lim_{N \to \infty} 1_N. \]

Similar bases can be constructed for fragmentations 2 and 3 as well.

We make the following approximation on Eq. (13)
\[ |\psi_1\rangle = G^{(l)}(z) v^{(s)} p P 1_N |\psi_1\rangle, \]
i.e. the operator \( v^{(s)} p P \) in the three-body Hilbert space is approximated by a separable form, viz.
\[ v^{(s)} p P = \lim_{N \to \infty} 1_N v^{(s)} p P 1_N \approx 1_N v^{(s)} p P 1_N \]
\[ \approx \sum_{n, \nu, \mu, \nu^{'}, \nu^{''}} | n \nu l \lambda \rangle \langle n \nu l \lambda | v^{(s)} p P | n \nu l \lambda \rangle \]
\[ \approx \sum_{n, \nu, \mu, \nu^{'}, \nu^{''}} | n \nu l \lambda \rangle \langle n \nu l \lambda | v^{(s)} p P | n \nu l \lambda \rangle , \]

FIG. 1: \( v^{(s)} \) and \( v^{(l)} \) for an attractive Coulomb potential.
where \( y_{1}^{(s)} = 1 (nu\lambda\nu_{1}^{(s)} pP|n' l' \lambda')_{1} \). Utilizing the properties of the exchange operator \( P \) these matrix elements can be written in the form \( z_{1}^{(s)} = p \times (-)^{l} 1 (nu\lambda\nu_{1}^{(s)}|n' l' \lambda')_{2} \).

With this approximation, solving Eq. (13) turns into solving the matrix equation

\[
(G^{(l)}(z))^{-1} - (\tilde{G})^{(s)} \bar{V} = 0
\]

for the component vector \( \bar{V} = 1 (nu\lambda|\nu_{1}) \), where \( G^{(l)} = 1 (nu\lambda C_{1}^{(l)}|n' l' \lambda')_{1} \). A unique solution exists if and only if

\[
D(z) = \det \{ (G^{(l)}(z))^{-1} - (\tilde{G})^{(s)} \} = 0.
\]

So, to calculate resonances, we need to search for the zeros of determinant \( D(z) \) on the complex energy plane.

The Green’s operator \( G^{(l)}(z) \) is related to the Hamiltonian \( H^{(l)}(z) \), which is still a three-body Coulomb Hamiltonian and seems to be as complicated as \( H \) itself. However this is not the case. The only possible two-body asymptotic configuration for \( H^{(l)}(z) \) is when particles 2 and 3 form a bound states and particle 1 is at infinity. The corresponding asymptotic Hamiltonian is

\[
\tilde{H} = H^{0} + v_{1}^{C}.
\]

Therefore, in the spirit of the three-potential formalism [5], \( G^{(l)}(z) \) can be linked to the matrix elements of \( \tilde{G}_{1}(z) = (z - \tilde{H})^{-1} \) via solution of a Lippmann-Schwinger equation,

\[
(G^{(l)}(z))^{-1} = (\tilde{G}_{1})^{-1} - U_{1},
\]

where \( \tilde{G}_{1} = 1 (nu\lambda|\tilde{G}_{1}|n' l' \lambda')_{1} \) and \( U_{1} = 1 (nu\lambda)(v_{2}^{(l)} + v_{3}^{C})(n' l' \lambda')_{1} \).

Now, what is remains is the calculation of the matrix elements \( \tilde{G}_{1} \), since the potential matrix elements \( y_{1}^{(s)} \) can always be evaluated numerically. The Green’s operator \( \tilde{G}_{1} \) is a resolvent of the sum of two commuting Hamiltonians, \( \tilde{H} = h_{x_{1}} + h_{y_{1}} \), where \( h_{x_{1}} = h_{x_{1}}^{0} + v_{1}^{C}(x_{1}) \) and \( h_{y_{1}} = h_{y_{1}}^{0} \), which act in different two-body Hilbert spaces. Thus, \( \tilde{G}_{1} \) can be given by a convolution integral of two-body Green’s matrices, i.e.

\[
\tilde{G}_{1}(z) = \frac{1}{2\pi i} \int_{C} \frac{dz' g_{x_{1}}(z - z') g_{y_{1}}(z')}{D(z')/D(z)dz} = N_{C'},
\]

where \( N_{C'} \) is the number of zeros inside the contour \( C' \). By calculating \( N_{C'} \) numerically we can decide whether a domain contains a resonance or not.

We considered the S-wave resonances of the \( e^{-} e^{-} e^{+} \) system. The resonances, found at the vicinity of thresholds, are seen in Fig. 3. The calculations were performed with three entirely different sets of parameters: \( x_{0} = 18 \) and \( y_{0} = 50 \), \( x_{0} = 25 \) and \( y_{0} = 50 \), \( x_{0} = 5 \) and \( y_{0} = 1000 \), while \( \nu = 2.1 \) in all cases (the lengths are given in \( a_{0} \) units). We found, that the results at \( N = 20 \) CS basis states and angular momentum channels up to \( l = \lambda = 10 \) are well converged and they are rather insensitive for the choice of CS parameter \( b \) over a broad interval. The resonances displayed in Fig. 3 are stable against the change of \( x_{0} \) and \( y_{0} \) parameters, they exhibit a remarkable 5 – 6 digits stability.

We can see that the resonances are aligned along a line pointing exactly to the two-body thresholds. As we stretched the code and went closer and closer to the threshold we discovered more and more resonances. All of them were along the line. This indicates that the two-body threshold is an accumulation point of the resonances, and probably there are infinitely many there.

This conclusion is supported by our previous study of the \( e^{+} + H \) system \( 7 \), where violent oscillations of the cross sections just above two-body thresholds were found. Preliminary resonance calculations with the present method show that in

\[FIG. 2: Analytic structure of \( g_{x_{1}}(E + i\epsilon - z') \) \( g_{y_{1}}(z') \) as a function of \( z' \). \( \epsilon = - \Gamma/2 \). The Green’s operator \( g_{y_{1}}(x) \) has a branch-cut on the \([0, \infty)\) interval, while \( g_{x_{1}}(E + i\epsilon - z') \) has a branch-cut on the \((-\infty, E + i\epsilon]\) interval and infinitely many poles accumulated at \( E + i\epsilon \) (denoted by dots). The contour \( C \) encircles the branch-cut of \( g_{y_{1}} \) such that a part of it goes on the unphysical Riemann-sheet of \( g_{y_{1}} \) (drawn by broken line) and the other part detoured away from the cut. The branch-cut and some poles of \( g_{x_{1}} \) (denoted by full dots) are lying on the physical Riemann-sheet, some other poles (denoted by empty dots) are lying on the un-physical Riemann-sheet of \( g_{y_{1}} \), respectively. Yet, the contour avoids the singularities of \( g_{x_{1}} \).
\]
FIG. 3: Accumulation of resonances above the two-body thresholds.

the $e^+ + H$ system, where the violent oscillations were found, there are also accumulation of resonances.

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