Accumulation of Three-Body Resonances above Two-Body Thresholds

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We calculate resonances in the three-body system with attractive Coulomb potential by solving homogeneous Faddeev-Merkuriev integral equations for complex energies. The equations are solved using the Coulomb-Sturmian separable expansion method. This approach allows us to study the exact behavior of the three-body Coulomb systems near the threshold. A negatively charged positronium ion is used as a test case. In addition to locating all previously known S-wave resonances of the positronium ion, we also find a large number of new resonant states that accumulate just slightly above the two-body thresholds. The pattern of accumulation of resonant states above the two-body thresholds suggests that probably they are infinite in number. We conjecture that this may be a general property of the three-body system with an attractive Coulomb potential.

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The common method for calculating resonant states in a quantum mechanical system is 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 has no effect on the discrete portion of the spectrum. At the same time, the branch cut in the complex energy plane, which corresponds to scattering states, is rotated, and the resonant states from the unphysical sheet become accessible.

In practice, the complex rotation technique is combined with a variational approach. The rotation in the complex energy plane turns the continuum into a set of discrete states. The points of the now discrete continuum scatter around the rotated-down straight line in the energy plane. It then becomes difficult, in particular, near the threshold, to decide whether a point is a resonant-state point or it belongs to the rotated continuum. A difficulty implicit in the variational calculation is related to the fact that the state is approached from above—hence, a resonance slightly above the threshold may easily evade detection.

Recently, we have developed a method for calculating resonances in the three-body Coulomb system by solving homogeneous Faddeev-Merkuriev integral equations [1] using the Coulomb-Sturmian separable expansion method [2]. As a test case, we calculated the resonances of the negative positronium ion. We also learned that in the case of attractive Coulomb interactions, Faddeev-Merkuriev integral equations may produce spurious resonances [3]. These spurious states can be singled out by varying the parameters introduced by the necessity of splitting the potential.

As we improved our skills in applying our method, more and more true new resonant states, all just slightly above the two-body thresholds, came to light. They are all aligned along a line in the complex energy plane pointing towards the two-body threshold. The pattern of accumulation of resonant states is very suggestive that there are infinitely many resonances all accumulating at the two-body threshold of the three-body Coulomb system. Since our method of calculation is relatively new we outline the basic concepts in the first part of the article. In the later part we explain the numerical techniques involved. Finally we specialize to the $e^-e^-e^+$ system and present our findings. For further details see Refs. [2,3].

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

$$H = H^0 + v_1^C + v_2^C + v_3^C, \tag{1}$$

where H^0 is the three-body kinetic energy operator. The potential v_α^C denotes the Coulomb potential in the subsystem α, where $\alpha = 1, 2, 3$. We use the usual configuration-space Jacobi coordinates x_α and y_α—coordinate x_α corresponds to pair (β, γ) and y_α connects the center of mass of (β, γ) to particle α. As a result, the potential v_α^C, between particles β and γ, depends only on the coordinate x_α.

The Hamiltonian (1) is defined in the three-body Hilbert space. The three-body kinetic energy after the center-of-mass motion is separated, is given by

$$H^0 = h^0_{x_\alpha} + h^0_{y_\alpha} = h^0_{x_\beta} + h^0_{y_\beta} = h^0_{x_\gamma} + h^0_{y_\gamma}, \tag{2}$$

where h^0 is the two-body kinetic energy. The two-body potential operators are formally embedded in the three-body Hilbert space as $v^C = v^C(x)\mathbf{1}_y$, where $\mathbf{1}_y$ 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 [1] the Coulomb interaction is split, in the three-body configuration space, into short-range and long-range

terms

$$v_\alpha^C = v_\alpha^{(s)} + v_\alpha^{(l)}, \tag{3}$$

where the short-range and the long-range parts are defined via a splitting function:

$$v_\alpha^{(s)} = v_\alpha^C \zeta(x_\alpha, y_\alpha), \tag{4}$$

$$v_\alpha^{(l)} = v_\alpha^C [1 - \zeta(x_\alpha, y_\alpha)]. \tag{5}$$

The splitting function ζ is defined such that

$$\lim_{x,y\to\infty} \zeta(x, y) = \begin{cases} 1, & \text{if } |x| < x_0(1 + |y|/y_0)^{1/\nu} \\ 0, & \text{otherwise} \end{cases} \tag{6}$$

where x_0 and y_0 are positive constants and $\nu > 2$. Therefore, in the region of the three-body configuration space where particles β and γ 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 $v_\alpha^{(s)} \sim 0$. It is common to use the functional form $\zeta(x, y) = 2/\{1 + \exp[(x/x_0)^\nu/(1 + y/y_0)]\}$. Typical forms of the short-range potential $v^{(s)}$ and the long-range potential $v^{(l)}$ are given in Fig. 1.

In a typical atomic three-particle system, two particles always have electrical charges of the same sign. Let us denote these two particles by 1 and 2; the third particle is denoted by 3. In this case the potential v_3^C is a repulsive Coulomb potential and it does not support two-body bound states. This means that the potential v_3^C can be considered as long-range potential. The Hamiltonian can then be written formally in a form which looks like a usual three-body Hamiltonian with two short-range potentials

$$H = H^{(l)} + v_1^{(s)} + v_2^{(s)}, \tag{7}$$

where the long-range Hamiltonian is defined as

$$H^{(l)} = H^0 + v_1^{(l)} + v_2^{(l)} + v_3^C. \tag{8}$$

The Faddeev method is now applicable. In this case it implies that the wave function can be written as a sum of two components

$$|\Psi\rangle = |\psi_1\rangle + |\psi_2\rangle. \tag{9}$$

The components are defined by $|\psi_\alpha\rangle = G^{(l)}(z) v_\alpha^{(s)} |\Psi\rangle$,

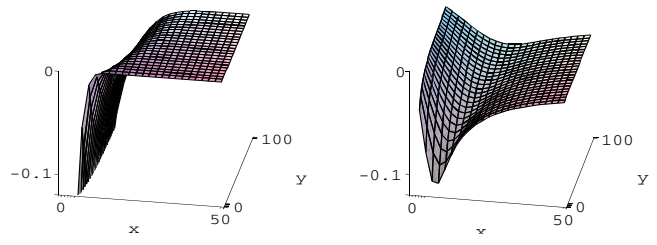

FIG. 1 (color online). The short-range and long-range potentials, $v^{(s)}$ and $v^{(l)}$, for an attractive Coulomb potential.

where $\alpha = 1,2$, $G^{(l)}(z) = (z - H^{(l)})^{-1}$, and z is a complex number.

In the case of the bound and resonant states the wave-function components satisfy the homogeneous, two-component Faddeev-Merkuriev integral equations

$$|\psi_1\rangle = G_1^{(l)}(z) v_1^{(s)} |\psi_2\rangle, \tag{10}$$

$$|\psi_2\rangle = G_2^{(l)}(z) v_2^{(s)} |\psi_1\rangle. \tag{11}$$

Equations (10) and (11) are valid for both, real and complex energies. The Green's function $G_\alpha^{(l)}$ is the resolvent of the channel long-range Hamiltonian: $G_\alpha^{(l)}(z) = (z - H_\alpha^{(l)})^{-1}$, where $H_\alpha^{(l)} = H^{(l)} + v_\alpha^{(s)}$.

Further simplification follows when we take into account the fact that particles 1 and 2 are identical and indistinguishable. For two identical particles, the Faddeev components $|\psi_1\rangle$ and $|\psi_2\rangle$, in their own natural Jacobi coordinates, have the same functional form. We use this fact to simplify the wave-function equations further. Let $\mathcal{P}$ be the permutation operator of particle indices 1 and 2. Its eigenvalues are $p = \pm 1$. We can write, $|\psi_2\rangle = p\mathcal{P}|\psi_1\rangle$. This implies that we can completely determine $|\psi_1\rangle$ from Eq. (10). Equation (10) now takes the form:

$$|\psi_1\rangle = G_1^{(l)} v_1^{(s)} p\mathcal{P} |\psi_1\rangle. \tag{12}$$

It is important to emphasize that Eq. (12) is exact. Despite the fact that the integral equation (12) has only one component, it correctly takes into account the complete asymptotic and symmetry properties of the system.

We solve Eq. (12), using the Coulomb-Sturmian separable expansion method. The Coulomb-Sturmian (CS) functions are defined by

$$\langle r|nl\rangle = \sqrt{n!/(n + 2l + 1)!}(2br)^{l+1} e^{-br} L_n^{2l+1}(2br), \tag{13}$$

where 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 $\{|nl\rangle\}$ form an orthonormal discrete basis in the radial two-body Hilbert space with respect to measure r^{-1}. For the ease of writing we define $\langle r|\widetilde{nl}\rangle = \langle r|nl\rangle/r$.

The three-body Hilbert space is a direct product of two-body Hilbert spaces. Therefore, an appropriate basis is simply the direct product of two, two-body angular momentum bases,

$$|n\nu l\lambda\rangle_1 = |nl\rangle_1 \otimes |\nu\lambda\rangle_1, \qquad (n, \nu = 0, 1, 2, \ldots), \tag{14}$$

where $|nl\rangle_1$ and $|\nu\lambda\rangle_1$ are associated with the coordinates x_1 and y_1, respectively. In this basis the completeness relation takes the form

$$\mathbf{1} = \lim_{N\to\infty} \sum_{n,\nu=0}^{N} |\widetilde{n\nu l\lambda}\rangle_{11} \langle n\nu l\lambda| = \lim_{N\to\infty} \mathbf{1}_1^N. \tag{15}$$

Next, we make the following approximation in Eq. (12)

$$|\psi_1\rangle = G_1^{(l)} \mathbf{1}_1^N v_1^{(s)} p\mathcal{P} \mathbf{1}_1^N |\psi_1\rangle. \tag{16}$$

In writing the Eq. (16) we approximated the operator $v_1^{(s)} p\mathcal{P}$ in the three-body Hilbert space by a separable form,

$$v_1^{(s)} p\mathcal{P} = \lim_{N\to\infty} \mathbf{1}_1^N v_1^{(s)} p\mathcal{P} \mathbf{1}_1^N \approx \mathbf{1}_1^N v_1^{(s)} p\mathcal{P} \mathbf{1}_1^N$$
$$\approx \sum_{n,\nu,n',\nu'=0}^{N} |n\widetilde{\nu l\lambda}\rangle_1 \underline{v}_1^{(s)} {}_1\langle n'\widetilde{\nu' l'\lambda'}|, \tag{17}$$

where $\underline{v}_1^{(s)} = {}_1\langle n\nu l\lambda | v_1^{(s)} p\mathcal{P} | n'\nu' l'\lambda'\rangle_1$. Utilizing the properties of the exchange operator $\mathcal{P}$ these matrix elements can be written in the form $\underline{v}_1^{(s)} = p \times (-)^{l'} {}_1\langle n\nu l\lambda | v_1^{(s)} | n'\nu' l'\lambda'\rangle_2$.

Approximations described by (16) and (17) enable us to turn the process of solving Eq. (12) into solving the matrix equation

$$\{[\underline{G}_1^{(l)}(z)]^{-1} - \underline{v}_1^{(s)}\} \underline{\psi}_1 = 0 \tag{18}$$

for the component vector $\underline{\psi}_1 = {}_1\langle n\widetilde{\nu l\lambda} | \psi_1\rangle$, where $\underline{G}_1^{(l)} = {}_1\langle n\widetilde{\nu l\lambda} | G_1^{(l)} | n'\widetilde{\nu' l'\lambda'}\rangle_1$. A unique solution exists if and only if Fredholm determinant of the system vanishes,

$$D(z) \equiv \det\{[\underline{G}_1^{(l)}(z)]^{-1} - \underline{v}_1^{(s)}\} = 0. \tag{19}$$

To determine the location of resonances, we need to search for the zeros of determinant $D(z)$ in the complex energy plane.

The Green's operator $\underline{G}_1^{(l)}$ is related to the three-body Coulomb Hamiltonian $H_1^{(l)}$. At first sight, the Hamiltonian $H_1^{(l)}$ appears to be as complicated as the original Hamiltonian H. However, closer inspection reveals that the only possible two-body asymptotic configuration for $H_1^{(l)}$ occurs when particles 2 and 3 form a bound state and particle 1 is at infinity. The corresponding asymptotic Hamiltonian is

$$\widetilde{H}_1 = H^0 + v_1^C. \tag{20}$$

Therefore, in the spirit of the three-potential formalism [4], the Green's function $\underline{G}_1^{(l)}$ is related to the matrix elements of the resolvent $\widetilde{G}_1(z) = (z - \widetilde{H}_1)^{-1}$ via solution of a Lippmann-Schwinger equation,

$$(\underline{G}_1^{(l)})^{-1} = (\widetilde{G}_1)^{-1} - \underline{U}_1, \tag{21}$$

where $\widetilde{G}_1 = {}_1\langle n\widetilde{\nu l\lambda} | \widetilde{G}_1 | n'\widetilde{\nu' l'\lambda'}\rangle_1$ and $\underline{U}_1 = {}_1\langle n\nu l\lambda | (v_2^{(l)} + v_3^C) | n'\nu' l'\lambda'\rangle_1$.

What remains now is to calculate the matrix elements $\widetilde{G}_1$. The Green's operator $\widetilde{G}_1$ is a resolvent of the sum of two commuting Hamiltonians: $\widetilde{H}_1 = h_{x_1} + h_{y_1}$, where $h_{x_1} = h_{x_1}^0 + v_1^C(x_1)$ and $h_{y_1} = h_{y_1}^0$. Two commuting Hamiltonians, h_{x_1} and h_{y_1} act in different two-body Hilbert spaces. Therefore, the operator $\widetilde{G}_1$ can be written as a convolution integral of two-body Green's matrices:

$$\widetilde{G}_1(z) = \frac{1}{2\pi i} \oint_C dz' \underline{g}_{x_1}(z - z') \underline{g}_{y_1}(z'), \tag{22}$$

where $g_{x_1}(z) = (z - h_{x_1})^{-1}$ and $g_{y_1}(z') = (z' - h_{y_1})^{-1}$. The contour of integration C is taken counterclockwise around the continuous spectrum of Hamiltonian h_{y_1} in such a way that the Green's function g_{x_1} is analytic on the domain encircled by C. The appropriate integration contour which satisfies the analyticity of Green's function g_{x_1} for resonant-state energies with $z = E - i\Gamma/2$ is depicted in Fig. 2.

The required CS matrix elements of the two-body Green's operators in the integrand are known exactly in analytic form for all complex energies (see [4] and references therein). From this follows that all thresholds that correspond to poles of $\underline{g}_{x_1}$ are at the right location irrespective of the value of N used in the separable expansion.

To calculate the energy of a resonant state we have to find a complex zero of the Fredholm determinant $D(z)$ of Eq. (19) near the branch cut. To achieve this goal we calculate the determinant $D(z)$ numerically along the real axis. We then use these numerically calculated values to form a Pade-type rational function approximation of $D(z)$. Next we look for zeros of the numerator polynomial. If a particular complex zero of the numerator polynomial is close to the real axis then $D(z)$ may have a zero on the second Riemann sheet. This signals that we should look for a complex zero in the neighborhood of this location. Here

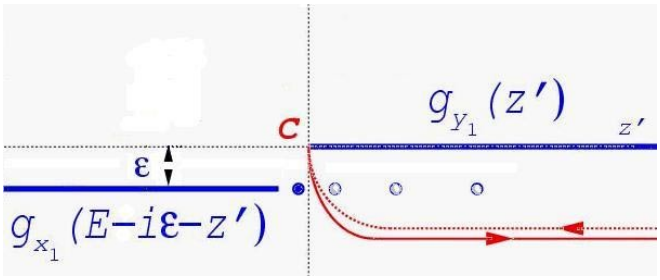

FIG. 2 (color online). Analytic structure of $g_{x_1}(E - i\varepsilon - z')g_{y_1}(z')$ as a function of z', $\varepsilon > 0$. The Green's operator $g_{y_1}(z')$ has a branch cut on the $[0, \infty)$ interval, while $g_{x_1}(E - i\varepsilon - z')$ has a branch cut on the $(-\infty, E - i\varepsilon]$ interval and infinitely many poles accumulated at $E - i\varepsilon$ (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} (indicated by the dotted line) and the other part detours away from the cut. The branch cut and some of the poles of g_{x_1} (depicted by dots) are lying on the physical Riemann-sheet. Other poles (depicted by circles) are lying on the unphysical Riemann-sheet of g_{y_1}. The contour as shown avoids the singularities of g_{x_1}.

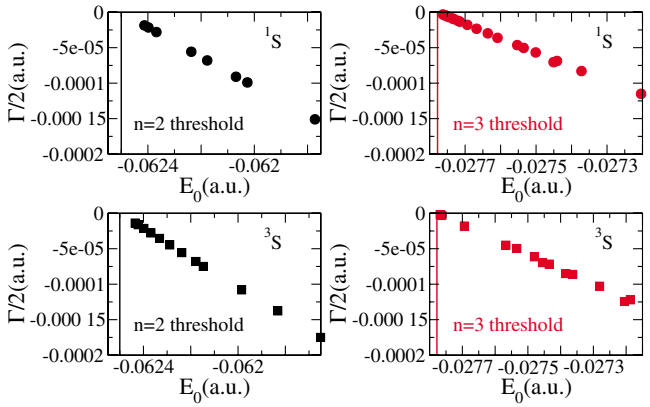

FIG. 3 (color online). Accumulation of resonances above the two-body thresholds. The energies are expressed in atomic units and measured from the three-body breakup threshold.

we used the method proposed in Ref. [5]. Pick three arbitrary complex points, z_1, z_2, and z_3 in such a neighborhood and calculate $f_1 = D(z_1)$, $f_2 = D(z_2)$, and $f_3 = D(z_3)$. The location z_4 of the complex root is estimated to be at the location given by

$$z_4 = \frac{z_1(z_2 - z_3)/f_1 + z_2(z_3 - z_1)/f_2 + z_3(z_1 - z_1)/f_3}{(z_2 - z_3)/f_1 + (z_3 - z_1)/f_2 + (z_1 - z_1)/f_3}. \tag{23}$$

We now make replacements: $z_1 \longrightarrow z_2$, $z_2 \longrightarrow z_3$, and $z_3 \longrightarrow z_4$, and calculate new z_4. This procedure is pursued until $D(z_4)$ becomes sufficiently small. The described operation is very fast, provided the initial values are close to some zero. In our case this condition is met. To be sure that we do not miss any zeros we use the *argument theorem* in complex analysis [6]. The number $N_{C'}$ of zeros of a function $D(z)$ *analytic* inside and on a simple closed curve C' in a complex plane is given by

$$\frac{1}{2\pi i}\oint_{C'} D'(z)/D(z)dz = N_{C'}, \tag{24}$$

where C' is the perimeter of the domain. To calculate integral of Eq. (24) we use the code NZERFZ from the CERN Program Library [7].

As an application and test case we considered the S-wave resonances of the well studied $e^-e^-e^+$ system [8]. Calculations were carried out 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 $y_0 = 1000$, and $\nu = 2.1$. We used a basis consisting of $N = 20$ CS radial states and angular momentum channels up to $l = \lambda = 10$. In all cases we found that the calculation converged well and that the results are insensitive to the choice of CS parameter b over a broad interval. In this case the basis for the separable expansion of the potential has $(N + 1)^2 \times (l_{\max} + 1) = 21^2 \times 11 = 4851$ elements. We also recalculated the resonance results with $N = 25$ basis states. We found numerical agreement to about 5–6 digits. The resonant energies are stable against the changes in x_0 and y_0 parameters. They also exhibit a remarkable 5–6 digits stability.

Using the new technique described in this Letter we have located all the previously known resonances of $e^-e^-e^+$ system. We also found several new resonances near the two particle threshold. Careful analysis of this energy region reveals that the systems posses a large number of such resonance states, (Fig. 3). All resonant states of the system lie along a line pointing toward the two-body threshold energy. This suggests strongly that the two-body energy threshold is the accumulation point of resonances.

This conclusion is also supported by our previous study of the $e^+ + H$ system [9]. In the study of $e^+ + H$ system we observed rapid oscillations of the scattering cross-section just above the $n = 2$ two-body threshold. Preliminary resonant-state calculations in the $e^+ + H$ system using the present method also suggests that resonant states are located at precisely those complex energies where the scattering cross section oscillates rapidly. As in the system presented in this article, resonant states appear to accumulate near the system two-body threshold. This strongly suggests that the appearance of the infinite number of resonant states near the two-body threshold is a general feature of the three-body system with attractive Coulomb interaction.

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