Accumulation of resonances in three-body Coulombic systems

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Abstract. We found that in three-body systems with attractive Coulomb potentials resonances accumulate at two-body thresholds from above.

We calculate resonances in three-body Coulombic systems by solving homogeneous Faddeev-Merkuriev integral equations. By investigating the negative positronium ion we located several 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.

In Merkuriev's approach [1] to the three-body Coulomb problem the Coulomb interaction is split in three-body configuration space into short- and long-range terms

$$v^C = v^{(s)} + v^{(l)}, \tag{1}$$

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

$$v^{(s)} = v^C\,\zeta(x,y) \qquad v^{(l)} = v^C\,[1-\zeta(x,y)], \tag{2}$$

x and y are the usual Jacobi coordinates. The splitting function ζ is defined such that

$$\lim_{x,y\to\infty}\zeta(x,y) = \begin{cases} 1, & \text{if } |x| < x_0(1+|y|/y_0)^{1/\nu}, \\ 0, & \text{otherwise,} \end{cases} \tag{3}$$

where $x_0, y_0 > 0$ and $\nu > 2$. So, in the region of three-body configuration space where two particles are close to each other $v^{(s)} \sim v^C$ and $v^{(l)} \sim 0$, otherwise $v^{(l)} \sim v^C$ and $v^{(s)} \sim 0$.

In the Faddeev approach we split the wave function into components, generally into three components. However, v_3^C, the potential between particles 1 and 2 (the two electrons), is repulsive and does not support bound states. Therefore the entire v_3^C can be considered as long range. This reduces the number of components to two. Further simplification can be achieved if we take into account that the two electrons 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

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hand $|\psi_2\rangle = p\mathscr{P}|\psi_1\rangle$, where $\mathscr{P}$ is the operator for the permutation of indices 1 and 2 and $p = \pm 1$ denotes the eigenvalue of $\mathscr{P}$. Therefore we can determine $|\psi_1\rangle$ from one equation only

$$|\psi_1\rangle = G_1^{(l)} v_1^{(s)} p\mathscr{P}|\psi_1\rangle, \tag{4}$$

where $G_1^{(l)}(z) = (z - H^0 - v_1^C - v_2^{(l)} - v_3^C)^{-1}$. This integral equation, although it contains only one component, yet gives a full account of both the asymptotic and symmetry properties of the system.

We solve Eq. (4) by using the Coulomb–Sturmian separable expansion approach (the details are given in Refs. [2, 3]). Within this approximation, Eq. (4) becomes a matrix equation for the component vector

$$\{[\underline{G}_1^{(l)}(z)]^{-1} - \underline{v}_1^{(s)}\}\underline{\psi}_1 = 0, \tag{5}$$

where $\underline{G}_1^{(l)}$ and $\underline{v}_1^{(s)}$ are the matrix elements of $G_1^{(l)}$ and $v_1^{(s)} p\mathscr{P}$, respectively, in the corresponding three-body Coulomb-Sturmian basis. A unique solution exists if and only if

$$D(z) \equiv \det\{[\underline{G}_1^{(l)}(z)]^{-1} - \underline{v}_1^{(s)}\} = 0. \tag{6}$$

To calculate resonances we have to find the complex zeros of the Fredholm determinant $D(z)$. Between thresholds $D(z)$ is analytic, therefore, due to a theorem of holomorphic functions [4],

$$\frac{1}{2\pi i}\oint_{C'} D'(z)/D(z)dz = N_{C'}, \tag{7}$$

where $N_{C'}$ is the number of zeros inside the contour C'. Thus, by calculating (7) 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. 1. 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). The resonances displayed in Fig. 1 are stable against the change of the parameters x_0 and y_0, 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 [5], where violent oscillations of the cross sections just above the two body thresholds were found. Preliminary resonance calculations with the present method show that in the e^+ + H system, where the violent oscillations were found, there is also an accumulation of resonances.

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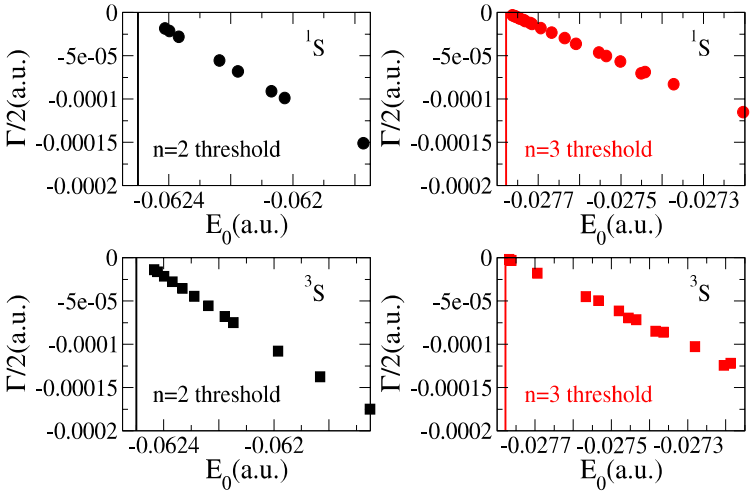

FIGURE 1. Accumulation of resonances above the two-body thresholds.

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