

Article

Resonances in Systems Involving Positrons

Anand K. Bhatia

Heliophysics Science Division, NASA/Goddard Space Flight Center, Greenbelt, MD 20771, USA;
anand.k.bhatia@nasa.gov

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Abstract: When an incident particle on a target gets attached to the target, the cross-section at that energy could be much larger compared to those at other energies. This is a short-lived state and decays by emitting an electron. Such states can also be formed by the absorption of a photon. Such states are below the higher thresholds and are called autoionization states, doubly excited states, or Feshbach resonances. There is also a possibility of such states to form above the thresholds. Then they are called shape resonances. Resonances are important in the diagnostic of solar and astrophysical plasmas. Some methods of calculating the resonance parameters are described and resonance parameters occurring in various systems are given.

Keywords: autoionization states; doubly excited states; Feshbach states; resonances; shape resonances

1. Introduction

In measuring scattering cross-sections, a peak or dip implies that the incident particle has formed a compound state which decays after a while. Such a state is called an autoionization state, a doubly excited state, or a resonance state, and has a very short lifetime compared to real bound states. Such states can also be formed by absorption of radiation in the target. Resonances are ubiquitous in electron-atom and electron-ion interactions. They play an important role in solar and astrophysical plasmas to infer temperatures and densities of plasmas [1]. However, they are not that common in the case of positron-target systems.

In a simple system like a positron-hydrogen, the positron and electron tend to be on the same side of the nucleus because of the attraction between the two particles, unlike in the case of the electron-hydrogen system where the two electrons tend to be on the opposite sides of the nucleus because of the repulsion between the two electrons. This shows that the correlations become very important in a positron-hydrogen system. This makes calculations of resonances difficult because many terms are required to calculate resonance parameters. Moreover, there is a positronium channel open below all the thresholds and this adds further complications.

2. Methods of Calculations

There are methods like the stabilization method, complex rotation method, Feshbach operator formalism [2], close-coupling method, and R -matrix method to calculate the resonance parameters. In approach [2], projection operators P and Q are defined such that P projects on a state and $Q = 1 - P$ removes that state, $P^2 = P$, $Q^2 = Q$ (idempotent), and $PQ = 0$ (orthogonality). We form a wave function $Q\Psi$ which is such that the lower states have been removed [3]. Therefore, using Raleigh–Ritz variational principle, we obtain eigenvalues:

$$\varepsilon_Q = \frac{\langle Q\Psi | H | Q\Psi \rangle}{\langle Q\Psi | Q\Psi \rangle} \quad (1)$$

These eigenvalues give us the positions of resonances. We obtain these bound states which are embedded in the continuum and are below the higher thresholds. They correspond to resonance states within the continuum which must be calculated separately and the width for each state must be calculated. In the narrow region of the width, the scattering phase shift increases by π radians. Calculation of the shift and width requires continuum functions (cf. Equation (2.13a)) in [3]. Various approximations like the exchange approximation, method of polarized orbitals, close-coupling approximation have been used to calculate continuum functions. However, it is difficult to write projection operators P and Q when the positronium channel is open. We need to use a method which does not depend on projection operator formalism [2].

The complex rotation method, based on a theorem by Belslev and Combes [4], has been applied extensively to calculate resonance parameters with great accuracy. The advantage of this formulation is that only discrete functions are included in the wave function and the continuum function is not necessary. In this method, the radial part is rotated by an angle θ . The Hamiltonian is transformed in the same way. The angle is varied until the eigenvalues do not change. Widths of the states are also obtained in the same calculation. Since there are also eigenvalues in the continuum, the shift mentioned above is included in the resonance positions obtained in this method. This is discussed further in Section 3.

This method gives the resonance positions which include the shift due to the interaction of discrete states with the continuum and need not be calculated separately. The eigenvalues obtained in this method are complex, where the complex part gives the width of the state.

In the positron-hydrogen system, Mittleman [5] showed that the equation for the positron-hydrogen system has an attractive potential proportional to $1/r^2$ due to the degeneracy of the $2s$ and $2p$ states of the hydrogen atom and therefore, there should be an infinite number of resonances in this case as in the electron-hydrogen system. Mittleman [5] conclusively showed the existence of resonances without carrying out detailed calculations. The resonances in electron-hydrogen system have been observed but not in the positron-hydrogen system, at least up to now.

3. Calculations and Results

The first successful calculation for the S -wave resonance was carried out by Doolen, Nuttal, and Wherry [6] using a sparse-matrix technique in the complex-rotation method. In this method, the radial coordinates are transformed by an angle θ :

$$r \rightarrow r e^{i\theta} \quad (2)$$

The Hamiltonian $H = T + V$ is transformed to:

$$H = T e^{-2i\theta} + V e^{-i\theta} \quad (3)$$

They used a wave function of the form:

$$\Phi(r_1, r_2, r_{12}) = \exp(-\alpha(r_1 + r_2)L_l^0(u)L_m^0(v)L_n^0(w) \quad (4)$$

In the above equation, α is the nonlinear parameter, L_l^0 is a Laguerre polynomial and:

$$u = \alpha(r_2 + r_{12} - r_1), v = \alpha(r_1 + r_{12} - r_2), \text{ and } w = 2\alpha(r_1 + r_2 - r_{12}) \quad (5)$$

They found only one resonance whose complex energy is given by:

$$E(\text{complex}) = \text{Re}(E) + \text{Im}(E) = \text{Re}(E) - i\Gamma/2 \quad (6)$$

$\text{Re}(E)$ represents the position of the resonance and the imaginary part represents the half width of the resonance. In this method, $\text{Im}(E)$ is plotted vs. $\text{Re}(E)$ and we look for the stationary paths as the

angle θ is increased for a fixed value of the nonlinear parameter α . Their results as a function of the number of terms are given in Table 1.

Table 1. Position and width of the resonance below $n = 2$ threshold of the hydrogen atom.

Number of Terms	Position	$\Gamma/2$
286	−0.2573744	0.0000676
364	−0.2573733	0.0000674
455	−0.2573745	0.0000671
560	−0.2573740	0.0000677
680	−0.2573741	0.0000677

This table shows that the resonance is at $E = -0.2573741$ Ry with a width of 0.0001354 Ry. It is clear from the table that a wave function with very large number of terms is needed to calculate the resonance parameters which is not so in the case of the electron-hydrogen. Prior to this, attempts by various authors failed to infer the existence of this resonance due to using a very small number of terms in their wave functions. This calculation provided incentive to look for resonances below the higher thresholds as well. Varga, Mitroy, Mezie, and Kruppa [7] carried out calculations below the $n = 2, 3$, and 4 thresholds. Their results are shown in Table 2. There are two resonances below $n = 2$ threshold, three below $n = 3$ threshold, and three below $n = 4$ threshold.

Table 2. Positron-hydrogen resonances [7] below higher thresholds. Units are Ry.

Threshold n	Position	Width
2	−0.257244	0.000132
	−0.250262	0.0000096
3	−0.116094	0.001284
	−0.112006	0.0003132
4	−0.076958	0.0000788
	−0.067714	0.0000528
	−0.064380	0.00003376

It is possible to find positions of higher resonances, using the relation between two resonances given by Temkin and Walker [8]:

$$\varepsilon_{n+1} = e^{-2\pi/\alpha} \varepsilon_n, \quad (7)$$

$$\alpha = (\sqrt{37} - 5/4)^{0.5} \quad (8)$$

This was deduced for electron-hydrogen resonances but does give reasonable values of higher resonances in positron-hydrogen system as well.

The potential between a positron and He^+ is repulsive. Therefore, an existence of resonances in this system seems unlikely. Using the stabilization method, Bhatia and Drachman [9] showed the existence of several resonances. This was confirmed by Ho [10] who carried out a definitive calculation using the complex rotation method described above and showed the correctness of their results [9]. Hylleraas type functions have been used in most calculations. The resonance parameters obtained by him are shown in Table 3.

Table 3. Positions and widths of S- and P-resonances in $e^+ - He^+$ system below the $n = 2$ threshold [10], Units Are Ry.

State	Position	Width
S-wave	-0.74099	0.25886
	-0.3712	0.0786
P-wave	-0.70869	0.35504
	-0.36956	0.08634

Kar and Ho [11] carried out similar calculations for $e^+ - He$ system and their results agree with those obtained by Ren, Han, and Shi [12], who used hyperspherical coordinates. Their results are shown in Table 4. The resonances are very narrow compared to those in $e^+ - He^+$ system.

Table 4. Resonance parameters in the $e^+ - He$ system. Units Are Ry.

Resonance	Ren, Han, and Shi [12]		Kar and Ho [11]	
	Position	Width	Position	Width
1	-4.15308	0.00046	-4.15306	0.00052
2	-4.13262	0.00030	-4.1326	0.00034
4	-4.12556	0.00004		

4. Resonances in Ps

The Ps^- system is obtained when the proton in H^- is replaced by a positron. Now the nucleus has the same mass as an electron. Therefore, the mass polarization term in the Hamiltonian becomes important. The binding energy of Ps^- is very close to half of the binding energy of H^- . The Hamiltonian is given by:

$$H = -2\nabla_1^2 - 2\nabla_2^2 - 2\nabla_1 \cdot \nabla_2 - 2/r_1 - 2/r_2 + 2/r_{12} \quad (9)$$

$$H = T + V \quad (10)$$

where r_1, r_2 , are the coordinates of electrons with respect to the positron and $r_{12} = |\vec{r}_1 - \vec{r}_{12}|$.

Resonances, in singlet and triplet states in Ps^- , have been calculated by Ho [13] using 364 terms in the singlet states and 455 terms in the triplet states. His results, obtained using the complex rotation method, are shown in Table 5.

Table 5. Singlet and triplet S-wave resonances in Ps^- . Positions are with respect to the ground state of the positronium. Units Are Ev.

<i>n</i>	Position	Width	Position	Width
			Singlet states	Triplet states
2	4.7340	1.17(-3)	5.0742	1.36(-4)
	5.0709	2.74(-4)		
3	7.7646	2.04(-3)	6.0038	2.72(-4)
	5.9908	1.50(-3)		
4	6.2526	3.27(-3)	6.3383	2.72(-4)
	6.3267	4.08(-3)		
	6.3317	4.63(-3)		
5	6.4519	6.12(-3)		
	6.4723	1.91(-3)		

There are several doubly-excited or Feshbach-type triplet *P* even parity resonances below $n = 2, 3, 4, 5$, and 6 thresholds. These have been calculated by Ho and Bhatia [14]. They are given below each threshold in Table 6. The third resonance below $n = 4$ threshold is a shape resonance because it is above the n threshold.

Table 6. Doubly-excited $^3P^e$ resonances in Ps^- .

n	Position (Ry)	Width (Ry)
2	-0.12440 ^a	0.00054
3	-0.063261	3.58(-4)
	-0.0562095	5.78(-5)
4	-0.037789236	3.01(-5)
	-0.0033087	1.8(-6)
	0-0.030972 ^a	6.4(-5)
5	-0.02493166	5.09(-5)
	-0.0220972	5.24(-5)
	-0.021660	2.64(-5)
6	-0.017596	1.06(-4)
	-0.015894	1.6(-4)
	-0.015811	1.14(-4)
	-0.013761	4.0(-5)

^a Shape resonance, above the threshold.

There are also odd parity triplet and singlet states which have been calculated by Bhatia and Ho [14–16]. Their results are shown in Tables 7 and 8. The lowest odd parity state in Ps^- has been observed by Michishio et al. [17] using laser beams of 2285 and 2297 angstroms and their results for the position and width agree with those given in Table 8.

Table 7. Odd parity triplet P-shape resonances of Ps^- .

n	State	Position (Ry)	Width (Ry)
3	^3P	-0.05450	9.20(-4)
5	^3P	-0.01971	6.60(-5)
7	^3P	-0.01008	4.00(-5)

Table 8. Odd parity singlet P-shape resonances of Ps^- .

n	Position (Ry)	Width (Ry)
2	-0.12434	9.00(-4)
4	-0.030975	6.00(-5)
6	-0.01375	5.20(-5)

Similar calculations have been carried out by Bhatia and Ho [18] for odd parity singlet and triplet D states of Ps^- . Their results are given in Table 9.

Table 9. Triplet and singlet D states of Ps^- . Positions are with respect to the ground state of $\text{Ps} = -0.5 \text{ Ry}$.

N	E(Ry)	Width (Ry)	E(Ry)	Width (Ry)
	Triplet States		Singlet states	
3	-0.05589808	3.12(-6)	-0.06008253	1.43(-4)
4	-0.034501270	3.61(-4)	-0.032722544	2.60(-5)
	-0.03269579	3.10(-5)	-0.037098862	4.78(-5)
			-0.032722544	2.60(-4)
			-0.0302010 ^a	8.54(-4)
5	-0.023408248	1.75(-4)	-0.2467214	4.60(-5)
	-0.01977681 ^a	8.14(-5)	-0.2191458	4.47(-5)
			-0.02135816	2.30(-4)

^a Shape resonance.

5. Resonances in PsH

As it is, it appears that the system having two neutral atoms, cannot have bound states. However, if it is viewed as a system consisting of a positron and H^- , then the positron is in the field of the Coulomb field of the hydrogen ion. There should be infinite number of bound states and resonances. Drachman and Houston [19] and Ho [20] have calculated the parameters of the S-wave resonance given below in Rydberg units:

$$E_R = -1.1726 \pm 0.0007 \quad \Gamma = (4.6 \pm 1.1) \times 10^{-6} \quad (11)$$

by Drachman and Houston [19], and:

$$E_R = -1.205 \pm 0.001 \Gamma = (5.5 \pm 2.0) \times 10^{-3} \quad (12)$$

by Ho [20].

Similarly, there are *P*-wave and *D*-wave resonances.

A hybrid theory [21] has been developed, which considers the long-range and short-range correlations at the same time. The theory is variationally correct. In the scattering calculations, calculated phase shifts have lower bounds to the exact phase shifts. This method has been applied to calculate resonance parameters in He and Li^+ . Phase shifts are calculated in the resonance region [22] and then fitted to the Breit–Wigner formula (cf. Equation (17) in [22]) to infer resonance parameters (cf. Equation (17) of [22]). The results obtained agree with those obtained using the Feshbach formalism [3]. The hybrid theory can also be applied to calculate resonance parameters in positron-target systems. Such calculations have not yet been carried out.

The books mentioned in references [1,23] have several chapters describing various methods employed to calculate resonance parameters. The author has two chapters in the book mentioned in ref. [1] (written with Aaron Temkin) on methods of calculating resonance parameters, also in [3].

6. Conclusions

Resonances in electron-target systems can be calculated easily. However, in the case of positron-target systems, calculations are not easy because of the positronium channel which is present below every threshold. As indicated above, correlations are very important. Therefore, wave functions having many terms are required. There are other systems with positrons where resonance parameters have been calculated. Here, we have discussed a few such systems and have described some of the methods of calculations. A theory called hybrid theory which includes the long-range and short-range correlations and is variationally correct has given resonance parameters for He and Li^+ , which agree with those obtained in earlier calculations. This is achieved by calculating phase shifts in the resonance region and fitting them to the Breit–Wigner expression to infer resonance parameters. This approach could be applied to positron-target systems. There could be results in the future, using this approach.

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